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(с соавторами и без)

I

СПИНОВЫЕ СИСТЕМЫ
ЭФФЕКТИВНЫЕ ПОТЕНЦИАЛЫ
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У 51 **Ульянов В.В**. Сборник обзоров и статей по квантовой теории (с соавторами и без). Часть I/ В.В.Ульянов. Электронное издание. - Х.: ХНУ имени В.Н.Каразина, 2011. - 84 с.

Сборник содержит несколько обзоров и статей, в которых затрагиваются различные вопросы квантовой теории. В первую часть входит один большой обзор, посвященный новым методам квантовой теории спиновых систем и так называемым квазиточнорешаемым моделям.

Он продолжает серию изданий, приуроченную к 200-летию Харьковского университета и 65-летию кафедры теоретической физики имени академика И.М.Лифшица.

Посвящается Льву Элеазаровичу Паргаманику – профессору кафедры теоретической физики, известному физику-теоретику, воспитавшему многих выдающихся специалистов.

Предназначен для научных работников, преподавателей, студентов и аспирантов физических специальностей вузов.

Издается по решению кафедры теоретической физики имени академика И.М.Лифшица от 17 мая 2011 года (протокол № 11)

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П Р Е Д И С Л О В И Е

В сборник включены некоторые обзоры и обзорные статьи, а также небольшие статьи, представляющие для автора особый интерес.

Большая часть этих публикаций написана совместно с моими колегами по кафедре теоретической физики.

Первая часть содержит только один большой обзор. Он обобщает результаты наших работ 1980-х годов по развитию новых методов исследования так называемых спиновых систем и обнаружению новых классов точных решений уравнения Шредингера, получивших название квазиточнорешаемых моделей, с помощью развитого *метода эффективных потенциалов*. Общие теоретические положения сопровождаются приложениями к конкретным спиновым системам.

Сборник посвящается Льву Элеазаровичу Паргаманику – профессору кафедры теоретической физики, известному физику-теоретику, воспитавшему многих выдающихся специалистов.

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На последней странице помещены изображения обложек физических журналов, в которых публиковались обзоры и статьи из данного сборника.

Благодарю Александра Михайловича Ермолаева за внимательное отношение к работам автора, за постоянную помощь советами и редкой литературой.

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New methods in the theory of quantum spin systems

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Contents:

Abstract:

Recently developed methods to investigate quantum spin systems are reviewed. These methods are based on somewhat unconventional applications of the spin coherent state technique developed in a series of papers in which the present authors were involved. A strict correspondence is shown to exist between energy spectra of a few spin and pseudospin systems and low-lying quantum states for a particle moving in a potential of a certain form. This suggests that quantum mechanical potential models have been found for which exact solutions are known for only a part of the spectrum (quasi-exactly solvable models). The properties of such models are discussed in detail. On the other hand, the above mentioned correspondence enables one to investigate low-temperature properties of anisotropic para- and superparamagnets. In this respect, the problem of tunnelling in such systems is of special interest. By means of the effective potential method, expressions for the tunnelling rate and metastable state decay at finite temperature are derived in a rather simple way. On a general basis an efficient potential description is developed also for some two- and many-particle systems (Dicke, Heisenberg, and Lipkin–Meshkov–Glick models). A Wigner–Kirkwood expansion of general form is constructed for spin systems of a general type. We also obtain energy quantization rules of the Bohr–Sommerfeld type with allowance for quantum corrections using an integral method and avoiding an approximate solution of the Schrödinger equation. We also discuss possible generalizations and perspectives of the methods discussed related to both group theoretical methods and applications of the quantum theory of magnetism.

1. Introduction

Spin systems are widespread in very different fields of physics, e.g., in the theory of magnetism, superconductivity, nuclear physics, etc. Special methods of theoretical physics are needed to describe the systems since commutation relations for spin components differ from the corresponding relations in both Bose and Fermi systems. As a rule, attention is mainly concentrated on the development of methods for many-particle systems, such as a Green function method, diagram technique, different representations of spin operators in terms of Bose operators [Mattis 1965, Akhiezer et al. 1968; White 1983; Baryakhtar et al. 1984; Kaganov and Chubukov 1987], etc. Meanwhile, until recently a series of one-spin Hamiltonians had remained essentially without investigation. In this connection, one could refer, for instance, to either anisotropic paramagnets or the asymmetric quantum top applied to the theory of molecule vibrations. It also concerns many-particle systems since in a few cases, e.g., small ferromagnetic particles, supermagnetism [Bean 1955; Bean and Livingston 1959], and the LGM model [Lipkin et al. 1965; Gilmore 1981], collective degrees of freedom are singled out describing the motion of the system as a whole.

In this review we develop mainly two directions in the investigation of such systems. On the one hand, we review papers where the strict potential field description of spin systems has been suggested (spin–coordinate correspondence). Such a correspondence, being based on the effective Schrödinger equation, turns out to be especially useful for studying quantum properties of these systems. On the other hand, a quasiclassical approximation is constructed for spin systems of general type (including many-particle ones), being convenient for finding quantum corrections and the energy quantization conditions when the behaviour of the quantum system is close to the classical one. Both methods (attributed partly to different limiting cases, and partly overlapping) are united by the fact that they are based on new applications of the spin coherent state technique [Radcliffe 1971; Perelomov 1972, 1986].

In its turn, the potential field method has two aspects for describing spin systems. On the one hand, it proves to be an obvious and efficient technique to study rather fine properties of spin systems, specifically, the behaviour of the magnetic susceptibility in the essentially quantum mechanical region, spin tunnelling, etc. On the other hand, the correspondence between spin and coordinate systems results in the discovery of new classes of exact solutions of the Schrödinger equation. The difference should be emphasized between the established exact spin–coordinate correspondence [Zaslavskii et al. 1983; Zaslavskii and Ulyanov 1984, 1987; Turbiner 1988a, b, c; Zaslavskii 1990a] and the spin variable technique conventionally used in the theory of magnetism to describe the dynamic interaction with allowance for the symmetry properties of the wave function, which concerns only coordinate degrees of freedom. The latter approach is approximate owing to one or another physical assumption: the possibility of averaging with respect to orbital variables, validity of perturbation theory, etc. A typical example is the derivation of the Heisenberg Hamiltonian which describes exchange effects in a hydrogen molecule [Heitler and London 1927]. The approach developed in the present paper is rigorous. In particular, the effective potential has been constructed for both the Heisenberg model and other spin systems with interaction (or systems which can be reduced to spin systems), for instance, the Dicke model for the atom–radiation interaction [Dicke 1954; Stenholm 1973].

One should dwell on the general question of exact solutions of the Schrödinger equation. Interest in

them has considerably increased recently. This is stimulated by the intensive development of group theoretical and algebraic methods of investigation. Among these are, for instance, the closely interrelated methods of supersymmetry [Witten 1981; Gendenstein 1983; Andrianov et al. 1984; Sukumar 1985], an application of the Darboux transformation [Zheng 1983, 1984], a factorization method [Infeld and Hull 1951; Mielnik 1984], and a method of finite-band potentials [Zaharov et al. 1980]. In a few papers [Alhassid and Iachello 1983; Alhassid et al. 1983, 1984, 1986; Wu et al. 1987] the dynamical symmetry of a series of potentials was studied using the angular momentum technique. As a result, one has succeeded both to figure out in more detail the algebraic nature of known exactly solvable models [Landau and Lifshitz 1977; Flügge 1971], and to find new ones (see also Ginnochio [1984, 1985] and Razavy [1980, 1981], where the exact solutions were found in a conventional manner).

The approach described here is yet another, new method of seeking for exact solutions. It is based on the consideration of Hamiltonians as functions of Lie group generators (in particular, of spin operators) and the use of the representation of generalized coherent states [Perelomov 1986, 1972]. In a relevant coordinate representation such a Hamiltonian becomes a differential operator, in particular, a Schrödinger operator with a certain effective potential energy. The characteristic feature of the method is its direct physical meaning since its underlying auxiliary structures, i.e. group Hamiltonians, by themselves describe various physical systems (see above).

The paper is organized as follows. In section 2 we develop a general technique of spin–coordinate correspondence related to the spin operator representation in differential form on the basis of spin coherent states. The effective Schrödinger equation is obtained and analysed with a symmetric and asymmetric potential well corresponding to a uniaxial anisotropic paramagnet (or superparamagnet) in an external magnetic field. On the basis of the potential field description the low-temperature magnetic properties of such a paramagnet are investigated. Analogous results are listed for a pseudospin model of Lipkin–Meshkov–Glick.

Exact solutions of the Schrödinger equation found on the basis of spin–coordinate correspondence are discussed. These solutions refer to $2S + 1$ energy levels (S being an integer or half-integer number entering the potentials and representing the spin value for a corresponding paramagnet). The potentials found are one- and two-parametric (at a fixed value of S). Their form and the structure of the energy spectrum substantially vary with the parameter values. In particular, a symmetric well and an asymmetric one with two minima are found, and also a well with a fourfold minimum. Simple analytical expressions are available for the uniaxial paramagnet, e.g., in the one-parameter case for $S = 0, 1/2, 1, 3/2$, and 2.

In section 3 periodic potentials are shown to correspond to a paramagnet with two axes. The spin system is characterized by (anti)-periodic solutions with the first energy levels in the $2S + 1$ lowest bands. New classes of exact solutions are found for energy bands with simple explicit expressions for the energy levels and wave functions for $S = 0, 1/2, 1, 3/2, 2, 5/2, 3, 7/2, 4, 9/2$, and 5. The potentials are expressed in terms of elliptic functions and contain in different particular cases a finite-band potential of Lame–Ince and Eckart and Morse. Rather interesting structural transformations are demonstrated to occur in the bands, in particular, band coupling.

Yet another approach to finding exact solutions of a similar type is considered, relevant to finite-dimensional three- and five-diagonal matrices. Using this approach, additional explicit solutions, being simple enough, are obtained. The most general structure leading to such solutions is discussed.

We also analyse a series of widespread physical models with an interaction of a different nature, viz., between fermions (LGM models), between a spin and a Bose mode, and between two different spins. The effective potential for them is constructed, and corresponding explicit solutions of the Schrödinger

equation [Turbiner and Ushveridze 1987; Turbiner 1988a, b, c] have a simple physical interpretation [Zaslavskii 1990d].

In section 4 the developed technique is applied to study tunnelling in spin systems. The problem of spin tunnelling is reduced to the problem of a particle moving in a two-well potential field. This allows one to introduce a simple and obvious definition of instanton in the spin system, and to calculate the level splitting due to tunnelling by conventional quantum mechanical methods [Zaslavskii 1990b]. Moreover, the structure of the energy spectrum is considered in a special region (in the vicinity of the potential barrier maximum) in which the spacing between pairs of levels is not exponentially small. The probability of metastable state decay at finite temperature is also calculated [Zaslavskii 1989, 1990c]. Tunnelling in many-body systems is discussed, in particular, in the Heisenberg model [Vekslerchik et al. 1989].

Section 5 is devoted to the construction of a quasiclassical approximation for spin systems. Using spin coherent states, an expansion of the Wigner–Kirkwood type is obtained [Zaslavskii 1984b], and applied later to the one-dimensional isotropic Heisenberg model [Zaslavskii 1987]. Using the number-of-states method [Ulyanov 1982], energy quantization rules of the Bohr–Sommerfeld type are found with the leading quantum correction taken into consideration. In the representation of spin coherent states, an exact closed equation is obtained for the mean value of an arbitrary function of spin operators, which is analyzed in several limiting cases [Zaslavskii 1984a; Zaslavskii et al. 1986].

In conclusion, different group theoretical aspects of the obtained results are discussed, as well as possible applications for other groups, for instance, SU(1, 1), and the possibility of generalization to multidimensional cases.

The present paper has two aspects and, accordingly, it could turn out to be useful mainly for two large groups of researchers. On the one hand, the methods suggested and the results obtained with them might be interesting for specialists in the field of the physics of magnetic phenomena, both for theorists and experimentalists. On the other hand, the questions considered in this review refer directly to quantum mechanics and new methods of mathematical physics.

2. The method of effective fields

2.1. Idea of the method. The effective potential of a uniaxial paramagnet

The spin represents a quantum mechanical object of essentially discrete nature. Therefore, for instance, the Schrödinger equation arising in the study of the energy spectrum of spin systems has a matrix form. As a rule, this makes the picture obscure and hampers the analysis of the spectrum by standard quantum mechanical methods. Here we demonstrate that for a sufficiently large class of spin systems a rigorous potential description can be introduced so that the energy spectrum of the spin system coincides with the $2S + 1$ (S being the spin value) energy levels for a particle moving in a potential field of sufficiently simple form. This results in a simple and obvious picture. Such a precise spin–coordinate correspondence serves as a basis for developing different approximate methods to describe the spin system, e.g., perturbation theory, quasiclassical approach, etc. For the coordinate system it suggests methods to find exact solutions of the Schrödinger equation.

Consider first the simplest case of a spin system described by a Hamiltonian corresponding to a paramagnet of the easy-axis type in a transverse magnetic field,

$$H = -\alpha S_z^2 - BS_x \,. \tag{2.1}$$

Here $\alpha > 0$ is the anisotropy constant, B is the magnetic field up to a constant factor.

Let us investigate the problem of finding the energy spectrum of such a system. In the S_z representation the wave function c_σ of the stationary state with energy E satisfies the difference equation

$$(E + \alpha\sigma^2)c_\sigma + \tfrac{1}{2}B\{[(S+\sigma)(S-\sigma+1)]^{1/2}c_{\sigma-1} + [(S-\sigma)(S+\sigma+1)]^{1/2}c_{\sigma+1}\} = 0 \,, \tag{2.2}$$

where the z-projections of the spin are denoted as $\sigma = -s, -s+1, \ldots, s$. Let us make the substitution

$$c_\sigma = a_\sigma \sqrt{(S-\sigma)!(S+\sigma)!} \,, \tag{2.3}$$

which allows us to eliminate the square roots, viz.,

$$(E + \alpha\sigma^2)a_\sigma + \tfrac{1}{2}B[(S-\sigma+1)a_{\sigma-1} + (S+\sigma+1)a_{\sigma+1}] = 0 \,. \tag{2.4}$$

As follows from these relationships, the generating function

$$\Phi = \sum_{\sigma=-S}^{S} a_\sigma \, \mathrm{e}^{\sigma x} \tag{2.5}$$

obeys the differential equation

$$\alpha\Phi'' - B \sinh x \, \Phi' + (E + BS\cosh x)\Phi = 0 \,. \tag{2.6}$$

Eliminating the term with the first derivative by introducing the function

$$\Psi = \Phi \exp[-(B/2\alpha)\cosh x] \,, \tag{2.7}$$

we come to the standard Schrödinger equation

$$\alpha\Psi'' + [E - (B^2/4\alpha)\sinh^2 x + B(S+\tfrac{1}{2})\cosh x]\Psi = 0 \,, \tag{2.8}$$

where x can be regarded as a certain dimensionless variable, and the solution $\Psi(x)$ decreasing at infinity can be regarded as a wave function. The anisotropy constant plays the role of the inverse particle mass.

Thus the problem of the eigenvalues and eigenvectors of the spin Hamiltonian $H = -\alpha S_z^2 - BS_x$ results in the coordinate picture of a particle moving in the effective potential field

$$U(x) = (B^2/4\alpha)\sinh^2 x - B(S+\tfrac{1}{2})\cosh x \,. \tag{2.9}$$

On the basis of the oscillation theorem for stationary bound states of one-dimensional Schrödinger equations, and owing to the absence of degeneracy of the energy levels in this case, one can come to the conclusion that the spin system energy values we are interested in coincide with the initial $2S + 1$ energy levels of the particle moving in the potential given by eq. (2.9). The higher energy levels have nothing to do with the spin system under consideration.

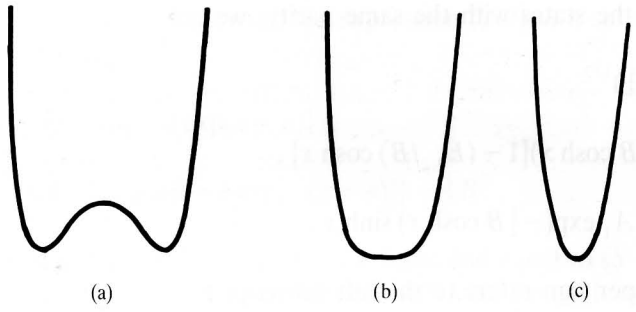


Fig. 1. The potential (2.9) for an easy-axis paramagnet in a transverse field.

Such systems with an "embedded" spectrum have been found in a series of papers [Razavy 1980, 1981; Zaslavskii et al. 1983; Zaslavskii and Ulyanov 1984, 1987; Zaslavskii 1990a; Turbiner and Ushveridze 1987; Turbiner 1988a, b, c]; a similar approach based on the introduction of the generating function has been developed in the papers of Scharf [1974, 1975] in his study of the Dicke model; it is being investigated intensively at present. The relation with other papers quoted and the history of this subject will be discussed in detail below at the end of section 3.

The found effective potential (2.9) undergoes a curious transformation as the magnetic field changes. For magnetic fields $B > B_0 = \alpha(2S+1)$ it has the form of single well (fig. 1c), while for $B < B_0$ it changes into a well with two minima (fig. 1a). It is especially interesting that the potential takes the form of well with a fourfold minimum (fig. 1b) at the critical magnetic field value $B = B_0$.

2.2. A class of exact solutions for symmetric potentials

In the class of problems under consideration, exact solutions, as was mentioned above, can be found for a limited number of excited energy levels. If the value of S is not too large, the wave functions and energy values have a simple explicit form, which is of special interest since usually the low-lying excited states can only be studied quantum mechanically (whereas for excited states a quasiclassical approach gives good results).

The sets of linear equations (2.2) and (2.4) can be split into two simpler ones since the states even in σ are separated from the odd ones. This simplifies the calculations significantly. For instance, for integer spin and even states we have $S+1$ equations instead of $2S+1$ ones. Consider the specific examples of the simple analytical expressions obtained for the energy levels and the stationary state wave functions (for simplicity, we shall use units in which $\alpha = 1$).

If $S = 0$ (this case is trivial for the spin system; however, in the coordinate picture the potential undergoes changes of a form typical for other values of S), then the ground state energy $E_0 = 0$ does not depend on B, and

$$\Psi_0 = A_0 \exp(-\tfrac{1}{2}B\cosh x)\,. \tag{2.10}$$

For the case $S = 1/2$ the corresponding quantities are

$$\begin{aligned} E_0 &= -\tfrac{1}{4} - \tfrac{1}{2}B\,, \qquad \Psi_0 = A_0 \exp(-\tfrac{1}{2}B\cosh x)\cosh\tfrac{1}{2}x\,, \\ E_1 &= -\tfrac{1}{4} + \tfrac{1}{2}B\,, \qquad \Psi_1 = A_1 \exp(-\tfrac{1}{2}B\cosh x)\sinh\tfrac{1}{2}x\,. \end{aligned} \tag{2.11a}$$

For $S = 1$, combining the states with the same parity, we get

$$E_{0;2} = -\tfrac{1}{2} \mp (B^2 + \tfrac{1}{4})^{1/2},$$

$$\Psi_{0;2} = A_{0;2} \exp(-\tfrac{1}{2} B \cosh x)[1 - (E_{0;2}/B) \cosh x], \tag{2.11b}$$

$$E_1 = -1, \qquad \Psi_1 = A_1 \exp(-\tfrac{1}{2} B \cosh x) \sinh x.$$

(Here and below the upper sign refers to the left subscript.)

The case $S = 3/2$ arouses special interest since it corresponds to the maximum number of exact solutions with a simple explicit form which describe completely enough the characteristic features of the energy spectrum. The solutions are

$$E_{0;2} = -\tfrac{5}{4} - \tfrac{1}{2} B \mp (B^2 - B + 1)^{1/2},$$

$$\Psi_{0;2} = A_{0;2} \exp(-\tfrac{1}{2} B \cosh x)[\cosh \tfrac{3}{2} x - (2/B)(E_{0;2} + \tfrac{9}{4}) \cosh \tfrac{1}{2} x],$$

$$E_{1;3} = -\tfrac{5}{4} + \tfrac{1}{2} B \mp (B^2 + B + 1)^{1/2}, \tag{2.11c}$$

$$\Psi_{1;3} = A_{1;3} \exp(-\tfrac{1}{2} B \cosh x)[\sinh \tfrac{3}{2} x - (2/B)(E_{1;3} + \tfrac{9}{4}) \sinh \tfrac{1}{2} x].$$

If $S = 2$, simple results can be be obtained for odd stationary states since the characteristic equation for this case is quadratic (whereas it is cubic for the even states),

$$E_{1;3} = -\tfrac{5}{2} \mp (B^2 + \tfrac{9}{4})^{1/2},$$

$$\Psi_{1;3} = A_{1;3} \exp(-\tfrac{1}{2} B \cosh x)[\sinh 2x - (2/B)(E_{1;3} + 4) \sinh x]. \tag{2.12}$$

The normalization factors in the above formulae can be expressed in terms of McDonald's functions. For example, for $S = 1/2$ they are

$$A_0 = [K_0(B) + K_1(B)]^{-1/2}, \qquad A_1 = [K_1(B) - K_0(B)]^{-1/2}.$$

It is curious that, although for the potential βx^4 exact solutions are known not to exist, they can be found for the case of the more complicated function $B_0^2 \sinh^4 \frac{1}{2} x$ (for low-lying states) corresponding to the critical field $B = B_0$.

2.3. *Some general properties of the energy spectrum*

Certain conclusions on the structure of the energy spectrum corresponding to the potential (2.9) for arbitrary value of S can be drawn if B is sufficiently large or small.

Consider first the former case. To begin with, let us stress that one cannot pass to the limit $B \to 0$ in eq. (2.9) immediately since the given potential is nonlocal and increases at infinity for arbitrarily small B.

To investigate small values of B (when the potential energy as a function of the coordinate has the

form of a double well), it is convenient to write the expression (2.9) as a sum of two Morse potentials with a constant additional term,

$$U(x) = (S + \tfrac{1}{2})^2\{\exp[2(x-a)] - 2\exp(x-a)\}$$
$$+ (S + \tfrac{1}{2})^2\{\exp[-2(x+a)] - 2\exp[-(x+a)]\} - \tfrac{1}{8}B^2 , \qquad (2.13)$$

where $a = \ln(2B_0/B)$. The depth of each well at $B = 0$ is finite and equal to $(S + 1/2)^2$. As $B \to 0$, in the first-order approximation the mutual influence of the wells can be neglected. In this limit, taking advantage of the known results for the Morse potential [Landau and Lifshitz 1977], we obtain

$$E_n = -(S - [n/2])^2 , \quad n = 0, 1, \ldots, n_{\max} , \qquad (2.14)$$

where the square brackets denote the integer part. If s is integer or half-integer, i.e., $n_{\max} = 2S$, then the corresponding states are spin states by their nature. The energy above values can be obtained directly from the spin Hamiltonian (2.1) for $B = 0$, so that the discrete spectrum turns out to be doubly degenerate except at the maximal spin level for integer S value. The levels $E > 0$ are relevant for the continuous spectrum.

Thus in the limit $B \to 0$, if S is integer, the spin part of the spectrum is directly connected with the continuous part. Note that for arbitrary and finite B it can be proved that the maximal spin level is $E_{2S} > 0$. In particular, it is always higher than the barrier separating the wells for $B < B_0$. On the other hand, if S is half-integer, then the spin part is separated from the continuous spectrum by an energy gap of finite width equal to $1/4$. For both cases all the spin levels are inside the potential wells, completely representing states of the discrete spectrum.

For the quasicontinuous "overspin" spectrum the quasiclassical quantization rules yield the following result as $B \to 0$:

$$E_n = \frac{\pi^2}{4}\,\frac{(n - 2S - \frac{1}{2})^2}{[\ln(B_0/B)]^2} , \quad n = 2S + 1, 2S + 2, \ldots . \qquad (2.15)$$

The values E_n for fixed n and $B \to 0$ tend to zero as the density increases.

The discrete nature of the overspin energy levels for small but finite B is one of the manifestations of the effect of the Morse wells on each other. This effect is reduced to potential decrease and tunnelling contact, as well as to a restriction of the range of the motion. The latter is not essential for negative energy levels, but for positive energy values it implies the transformation of the spectrum from continuous to discrete. It should be noted that expression (2.15) for the energy levels refers to motion in an infinitely rectangular potential well with a width $\sim\ln(B_0/B)$.

Next, let $B \to \infty$. Rewrite the potential (2.9) as follows:

$$U(x) = -B(S + \tfrac{1}{2}) + \tfrac{1}{4}B^2(\sinh^2 x - x^2) - B(2S + 1)\sinh^2 \tfrac{1}{2}x + \tfrac{1}{4}B^2x^2 .$$

As $B \to \infty$, the contribution of the two last terms can be calculated by means of perturbation theory. As a result, we get a "fan" of levels with a linear dependence on B,

$$E_n = (n - S)B + \tfrac{1}{2}n^2 - (n + \tfrac{1}{2})S + O(B^{-1}) , \quad n = 0, 1, \ldots .$$

This formula is relevant to both spin and overspin states. It can be derived from the spin Hamiltonian using perturbation theory with further extension to $n > 2S$.

It should be stressed that the behaviour of the energy spectrum considered in this section is not related to the existence of exact solutions for integer or half-integer S, i.e. to the existence of a spin–coordinate correspondence. The characteristic division of the spectrum in discrete and quasidiscrete parts as $B \to 0$ exists for any value of $S \geq 0$ (for negative values, $S < 0$, there are no discrete levels).

The change of the form of the potential and of the behaviour of the energy spectrum referred to above will be shown below to lead, for the relevant spin systems, to such physical results as, for instance, the existence of a maximum of the low-temperature magnetic susceptibility as a function of magnetic field.

2.4. *A class of asymmetric potentials*

The results obtained in the preceding section can be generalized to the case of potential fields of the form

$$U(x) = \tfrac{1}{4}B^2(\sinh x - C/B)^2 - B(S + \tfrac{1}{2})\cosh x\,, \tag{2.16}$$

which, in contrast to eq. (2.9), are asymmetric; for fixed S they contain two variable parameters, $B > 0$ and $C > 0$. Meanwhile, wave functions of the first $2S + 1$ levels have a form which differs from eqs. (2.6) and (2.7) by the factor of $\exp(\frac{1}{2}Cx)$, and the quantities c_σ satisfy an equation analogous to eq. (2.2) with the only difference that the factor before c_σ contains the additional term σC.

In the present case, the potential profile is essentially different depending on whether, on the plane of the parameters B and C, the point corresponding to the system lies inside, outside or on the astroid $B^{2/3} + C^{2/3} = B_0^{2/3}$. In the first case, the potential represents a well with two minima (fig. 2a), in the second one the potential well has one minimum (fig. 2c), and in the third case the maximum and the

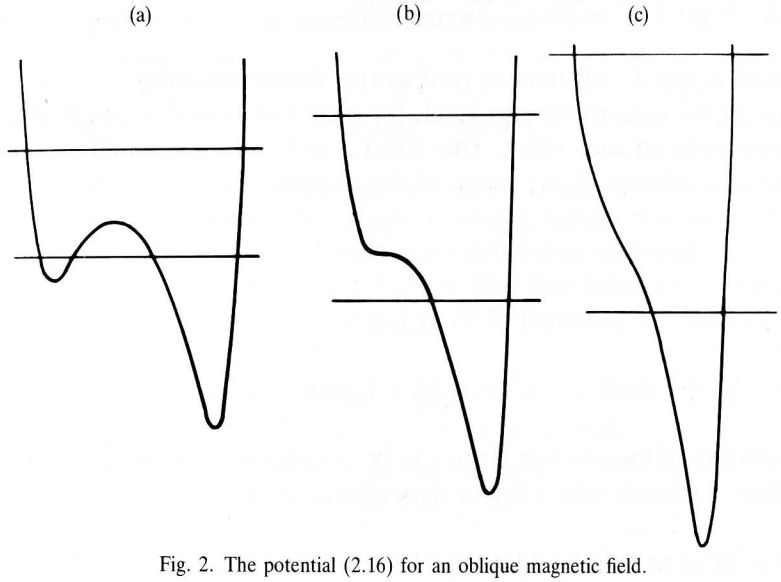


Fig. 2. The potential (2.16) for an oblique magnetic field.

nearest minimum merge resulting in an inflection point with a horizontal tangent (fig. 2b). The point $C = 0$, $B = B_0$ on the astroid corresponds to the critical field value for the symmetric case.

It is interesting that the above mentioned potential profile deformation is a typical example of the transformations which are analysed in catastrophe theory, namely a cusp catastrophe, the simplest realization of which is in a so-called Ziman machine [Poston and Stewart 1978].

The potential (2.16) refers to the dimensionless spin Hamiltonian

$$H = -S_z^2 - BS_x - CS_z\,, \tag{2.17}$$

which describes an anisotropic easy-axis paramagnet, where B and C are proportional to the transverse and longitudinal magnetic field components, respectively. The cited equation of the astroid is a quantum mechanical generalization of the equation distinguishing the metastable state region for such a paramagnet in the classical case [Landau and Lifshitz 1982, section 41].

In contrast to eq. (2.2), in the present characteristic equation the states even in σ do not separate from the odd ones, so that the order of the equation equals $2S + 1$. We list simple exact solutions for $S = 0$ [when the potentials (2.9) and (2.16) have a form related to supersymmetric quantum mechanics] and $S = 1/2$. For the former case,

$$E_0 = 0\,, \qquad \Psi_0 = A_0 \exp(-\tfrac{1}{2}B\cosh x + \tfrac{1}{2}Cx)\,, \tag{2.18a}$$

and for the latter case,

$$E_{0;1} = -\tfrac{1}{4} \mp \tfrac{1}{2}(B^2 + C^2)^{1/2}\,,$$
$$\Psi_{0;1} = A_{0;1} \exp(-\tfrac{1}{2}B\cosh x + \tfrac{1}{2}Cx)\left[\mathrm{e}^{x/2} - \mathrm{e}^{-x/2}\left(\frac{C \mp (B^2 + C^2)^{1/2}}{B}\right)\right]. \tag{2.18b}$$

Note that the special functions closest to the solutions considered for $C = 0$ are the Coulomb spheroidal functions [Abramowitz and Stegun 1964; Komarov et al. 1976]. On the other hand, the case $C \neq 0$ yields one of the generalizations of this kind of special functions.

The energy spectrum has a series of interesting properties absent in the case of the symmetric potential (2.9). These properties are most pronounced in the limit $B = 0$. Let us consider it in more detail. First, note that the potential energy (2.16) can be written (for arbitrary values of B and $C < B_0$) as a sum of two Morse wells (up to a constant additional term),

$$U = \tfrac{1}{4}(B_0 + C)^2(\mathrm{e}^{2(x-b)} - 2\,\mathrm{e}^{x-b}) + \tfrac{1}{4}(B_0 - C)^2(\mathrm{e}^{-2(x+a)} - 2\,\mathrm{e}^{-(x+a)}) + \tfrac{1}{4}C^2 - \tfrac{1}{8}B^2\,,$$

localized near the points

$$x = b = \ln\frac{2(B_0 + C)}{B}\,, \qquad x = -a = -\ln\frac{2(B_0 - C)}{B}\,.$$

In the limiting case $B = 0$ we obtain for $C < B_0$ two solitary Morse wells (plus a term $C^2/4$). The energy spectrum consists of the combined energy levels of the separate wells, the exact solutions being

obtained for arbitrary $C < B_0$ and not only for spin values of the parameter S. For example, for the right-hand larger well

$$E_k = -(S-k)^2 - C(S-k), \quad k = 0, 1, \ldots, N-1, \tag{2.19}$$

where N indicates the number of levels equal to the integer nearest to $N_0 = S + C/2 + 1$, for which $N < N_0$.

If $C = 0$, the wells are equal. As C increases, the number of levels also increases for the right-hand well and decreases for the left-hand one. For $C = 2S$ the smaller well loses all its levels and disappears itself at $C = 2S + 1$. In the pre-critical region $C \leq 2S + 2$ the total number of bound states is conserved, and starting from $C > 2S + 2$, a new phenomenon emerges, viz. the overspin levels are "dragged" into the remaining well. Meanwhile, all the levels have the energy values described by formula (2.19) with $k \geq 2S + 1$ for the overspin states. In a plot of $E_n(C)$ the new overspin levels start from the point where the straight lines (2.19) are tangent to the parabola of the continuous spectrum boundary $C^2/4$.

Let us pay attention to the peculiar behaviour of the levels $E_n(C)$. In the point relevant to integer values $C \leq 2S$ levels are exchanged between the wells, not only at the outlet of the well, but also in the middle of the spectrum. The greatest number of "exchange processes", equal to $2S$, is due to the maximum spin level, and the smallest number is due to the ground state (no exchange). For all the levels except the maximum one, each exchange is accompanied by a transition from one fixed S_z to another. It results in a broken behaviour of all the levels $E_n(C)$ except the ground state, whose energy decreases monotonically as C increases: $E_0 = -S^2 - CS$. The above mentioned exchange processes occur for such values of C that all the discrete levels are spin levels; they result in the transition of levels to the deeper well.

Thus, the potential (2.16) allows exact solutions for integer and half-integer S and, in addition, has a series of curious properties as $B \to 0$. Let us enumerate them once more: a very simple exact solution for the energy levels for all S (including non-spin values) throughout the whole range of C; energy level exchange between the wells; overspin bound states emerging for $C > B_0 + 1$; monotonic decrease of the ground state energy level and broken behaviour of the other levels.

Note that, since the breaks of $E_n(C)$ refer to excited states, there are no low-temperature discontinuities of the magnetization (whereas there are discontinuities for the spin Hamiltonian of the "easy-plane" type [Filatova and Tsukernik 1969; Rosenfeld 1976] since the ground level has been proved to have broken behaviour).

If a small but finite B is introduced, then the degeneracy is removed and the levels coinciding at $B = 0$ become mutually repulsive.

For the behaviour of the spectrum in strong fields, there is a typical linear dependence of the energy levels on the "intensity" $(B^2 + C^2)^{1/2}$ [compare with an analogous result for the potential (2.9) pointed out at the end of the relevant section].

Let us emphasize now the following differences between the classes of potential fields considered above and the standard exactly solvable models known from quantum mechanics [Landau and Lifshitz 1977; Flügge 1971]. First, the latter are actually one-parametric. They can be written in the form $U(x) = U_0 f(x/a)$. When the parameter U_0 is changed, the "intensity" (but not the form) of the potential changes. To these models belong, for instance, the Eckart potential, $-U_0/\cosh^2(x/a)$, and the Morse potential, $U_0[\exp(-2x/a) - 2\exp(-x/a)]$, etc. On the other hand, power models (such as the harmonic oscillator, quartic oscillator, or linear potential) actually do not contain any parameter, since the Schrödinger equation in terms of dimensionless parameters takes the form

$$\Psi'' + (E - x^m)\Psi = 0 .$$

Meanwhile, the spin-type models considered here have much richer possibilities. So, the potential form can change essentially even in the one-parametric case, i.e., when $C = 0$ (see fig. 1). As for the models with $C \neq 0$ leading to a two-parametric (for fixed S) potential (see fig. 2), they seem to have no analogues in the above mentioned sense among the standard models.

Secondly, in the case at hand the spectrum is completely discrete and the potentials have no singularities. In this respect, the symmetric potentials found could be compared partly with only one exactly solvable model, specifically, the harmonic oscillator. However, as has already been pointed out, the profile of the latter is fixed in contrast to the examples considered in this paper, and the structure of the energy spectrum is monotonic.

2.5. *Periodic potentials with exact solutions*

We have considered so far the Schrödinger equation for potential wells, the discrete spectrum being obtained as a result of the wave function's decreasing at infinity. It turns out that there also exist a class of periodic potentials which allow exact solutions and have a direct relationship to the spin system. The relevant Schrödinger equation reads

$$\frac{d^2\Psi}{d\varphi^2} + [\kappa - \tfrac{1}{4}B^2 \sin^2\varphi - B(S + \tfrac{1}{2}) \cos\varphi]\Psi = 0 . \tag{2.20}$$

It can be derived from eqs. (2.8) and (2.9) through the formal substitution $x \to i\varphi$. The wave functions for the energy values attributed to the energy spectrum of the relevant spin systems read

$$\Psi(\varphi) = \exp(-\tfrac{1}{2}B \cos\varphi) \sum_{\sigma=-S}^{S} \frac{c_\sigma}{\sqrt{(S-\sigma)!(S+\sigma)!}} \exp(i\sigma\varphi) , \tag{2.21}$$

where c_σ satisfy the relationships (2.2). These solutions obey periodic or antiperiodic boundary conditions (here and below we shall speak simply about a periodic potential without reference to the specific form of the boundary conditions; it should be noted that for $S = -1/2$ eq. (2.20) reduces to a Mathieu equation) depending on S,

$$\Psi(\varphi + 2\pi) = (-1)^{2S}\Psi(\varphi) . \tag{2.22}$$

The above considered energy values E of the spin system (viz., the easy-axis paramagnet) differs only in sign from the corresponding eigenvalues of eq. (2.20): $E = -\kappa$. In other words, their arrangement in the spectra is reversed. For $S = 0$, $1/2$, 1, $3/2$, and 2 the explicit expressions for the eigenvalues κ and eigenfunctions $\Psi(\varphi)$ are similar to those listed in section 2.2 (with a change of the level numbering and the sign of the energy and replacement of hyperbolic functions by trigonometric ones). On the other hand, these eigenvalues coincide both in value and in sign with the spectrum of the spin Hamiltonian of the "easy-plane" type $H = \alpha S_z - BS_x$.

Due to the symmetry properties of the potential, one can turn from eq. (2.22) to more conventional boundary conditions. For instance, for the case of odd states and integer spin, one gets the problem of a particle moving at $0 \leq \varphi \leq \pi$ in a potential well with boundary conditions $\Psi(0) = \Psi(\pi) = 0$. (An

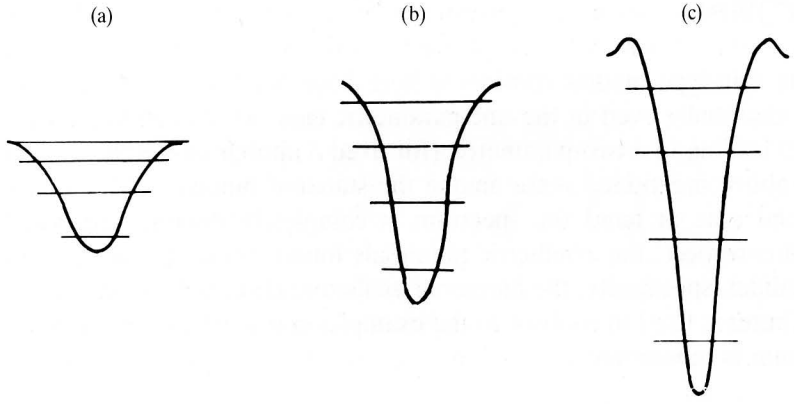


Fig. 3. The potential for the easy-plane case.

analogous procedure can be performed for other cases.) Such a reformulation of the boundary conditions allows one to classify the energy levels using an oscillation theorem, from which, on the basis of the specific form of the wave function, it follows that the first $2S + 1$ values of κ correspond to the spin system.

The obtained solutions allow a simple interpretation in terms of an energy band diagram: They correspond to quasimomentum $K = 0$ if the spin is integer, and to $K = 1/2$ if the spin is half-integer. In the picture of reduced bands, the alternating bottom and top of different bands correspond to "energy" values. For $B = 0$ one gets the conventional problem of a planar free rotator for integer S and a rotator with antiperiodic boundary conditions for half-integer S.

The spectrum of the Schrödinger equation (2.8) contains an infinite number of levels, the extra (with respect to the spin system) energy values being positioned above E_{2S}. The spectrum of eq. (2.20) with the indicated boundary conditions also contains an infinite number of levels; however, their arrangement is reversed owing to $E = -\kappa$. To the value E_0 of the ground state energy of the spin system (we refer to an "easy-axis" paramagnet) corresponds κ_{2S}, and the extra energy values are positioned below E_0. The $2S + 1$ levels which are the intersection of both sets correspond to the spin system.

In fig. 3, the behaviour of the potential is plotted for $S = 3/2$ for the cases $B = 2$ (fig. 3a) and $B = 4$ (fig. 3b), when the potential has a fourfold maximum, and $B = 6$ (fig. 3c); the energy spin levels are also shown.

An equation with a complex periodic potential corresponds to a spin system with an oblique field ($C \neq 0$), and the condition

$$\Psi(\varphi + 2\pi) = \exp[\mathrm{i}(\tfrac{1}{2}S - C)2\pi]\Psi(\varphi)$$

singles out real energy values from the band solution. For $S = 0$ and $1/2$ especially simple exact solutions can be obtained, analogous to those listed in section 2.2.

2.6. Low-temperature magnetic properties of a uniaxial paramagnet

In this section we apply the technique developed in sections 2.1–2.5 to the analysis of the magnetic properties of a spin system with Hamiltonian (2.1). The corresponding physical object is, for instance, a magnetic dissolved crystal, viz. transition group ions in paramagnetic salts. The structure of the part of

energy spectrum of such a system that corresponds to the energy splitting of the ground state of the paramagnetic ion by the crystal field can be well described by an effective spin Hamiltonian [White 1983].

A superparamagnet, whose total magnetic moment is made up of a macroscopic number of magnetic electron spins [Bean 1955; Bean and Livingston 1959], is another example.

The effective potential method adequately fits the determination of the magnetic field dependence of the energy, magnetization, and ground state susceptibility for the following reason. In the study of low-temperature properties of magnetic systems described by spin quantum models, a semiclassical approach is often used. One considers small oscillations of the magnetization against the background of the equilibrium configuration found by classical methods, i.e., the Hamiltonian of the spin system is replaced by the Hamiltonian of a system of harmonic quantum oscillators through the transition to Bose creation and annihilation operators.

Such a procedure allows one to investigate a wide range of magnetically ordered systems, for both equilibrium and nonequilibrium conditions [Akhiezer et al. 1968]. In particular, if the external magnetic field is directed along the easy axis of anisotropy of a uniaxial crystal, then the ground state energy and spin wave spectrum found in a semiclassical way precisely coincide with the true quantum values for an arbitrary atomic spin value [Mattis 1965].

If the external field is orthogonal to the anisotropy axis (as in the case under consideration), then generally speaking, the energy values cannot be found exactly, and the above mentioned semiclassical treatment results in a series of contradictions. One of them is that in the low-temperature range, for field strengths somewhat lower than critical, which is the field strength at which the classical spin becomes directed along the field, the transverse magnetization within this approach turns out to be larger than the maximum allowed one [Turov 1963]. This contradiction is not related to the fact that the system considered in the cited paper is magnetically ordered: In the absence of exchange interaction a semiclassical calculation results even in an infinite magnetization in a field equal to the critical one [Filatova and Tsukernik 1967].

In the latter case, the reason of the emerging contradictions is that actually, at field strengths sufficiently close to critical, the energy spectrum is essentially restructured, which cannot be described by the above mentioned approximation. Therefore, a more consistent treatment of specific quantum effects is needed, which is most naturally and simply performed, as we shall see, by the effective potential method.

First, let us call the results of the classical approach [Landau and Lifshitz 1982], in which S_i ($i = x, y, z$) are regarded as c-number components of a vector of length S. For fields not exceeding the critical value $2S$, there are two equilibrium directions symmetric with respect to the x-axis, while the magnetization along this axis increases linearly with the field strength. Starting from the value $B = 2S$, the spin turns out to be directed along the x-axis, i.e. saturation is achieved. Thus, when the field strength becomes equal to critical, the magnetization (in a classical treatment) undergoes an abrupt change and the susceptibility has a discontinuity. However, according to quantum mechanics, whatever finite values the magnetic field achieves, the magnetization $\langle S_x \rangle$ cannot achieve a spin value S, since S_x has no definite value in the stationary state of the system described by the Hamiltonian (2.1). The system properties change smoothly.

Let us turn to a consistent quantum mechanical treatment. As follows from eq. (2.2), $c_{-\sigma} = \pm c_\sigma$ and, consequently, the probability distribution function for S_z is even with respect to σ. Therefore, $\langle S_z \rangle = 0$ in stationary states. As follows from symmetry arguments, $\langle S_y \rangle = 0$ in these states as well. Thus, only the mean value of the spin projection on the x-axis is nonzero. It can be found by differentiating the energy with respect to the parameter B, i.e., $\langle S_x \rangle = -\partial E / \partial B$.

Energy level values can be found as solutions of characteristic equations written, for instance, using a terminating continued fraction. For example, for the integer spin case of odd states, the equation in the corresponding standard notation for such fractions reads

$$E + S^2 - \frac{1 \cdot 2S(\frac{1}{2}B)^2|}{|E + (S-1)^2} - \cdots - \frac{n(2S-n+1)(\frac{1}{2}B)^2|}{|E + (S-n)^2} - \cdots - \frac{(S-1)(S+2)(\frac{1}{2}B)^2|}{|E+1} = 0 . \qquad (2.23)$$

Analogous equations can also be derived in other cases.

For spins $S = 1/2$, 1, and $3/2$ the energy levels, as well as the magnetization and susceptibility, can be calculated exactly. They have a simple form [see eq. (2.2)]. As for spins $S = 2$, $5/2$, and 3, we have found these quantities for the ground state through a numerical calculation based on equations of the type (2.23). In fig. 4 we demonstrate the typical smooth behaviour of the magnetization compared with the broken classical behaviour (for the case $S = 3$). The typical dependences plotted in fig. 5 for the ground state susceptibility $\chi = 2(\mathrm{d}/\mathrm{d}B)\langle S_x \rangle$ against the field intensity (the factor of 2 is introduced for convenience) are essentially different from the classical step-like dependence.

In the ranges of very weak and extremely strong field intensities, the results for arbitrary spin can be obtained using standard perturbation theory or directly from equations of the type (2.23). The expressions corresponding to the ground state susceptibility read

$$\chi = \frac{S}{S-\frac{1}{2}} + \tfrac{3}{16}B^2 \frac{S}{(S-\frac{1}{2})^3(S-1)} , \quad B \ll B_0/\sqrt{S}, S > 2 , \qquad (2.24)$$

$$\chi = \frac{S(S-\frac{1}{2})}{B^3} , \qquad B \gg B_0 . \qquad (2.25)$$

According to formula (2.24), the susceptibility increases for weak fields, while it rapidly decreases for strong fields, as can be seen from eq. (2.25). This leads to a conclusion for the behaviour of the ground state susceptibility, with the results for spins $S = 1$, $3/2$, and 2 taken into account. If $S = 1$, then

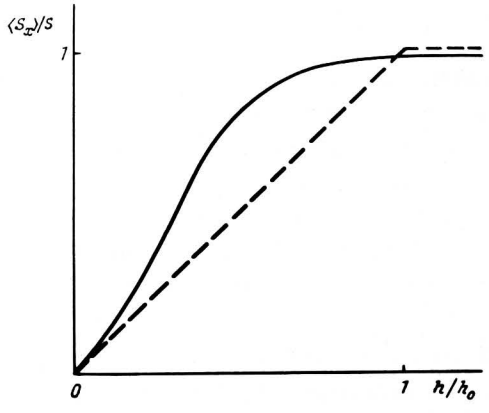


Fig. 4. The field dependence of the magnetization for $S = 3$.

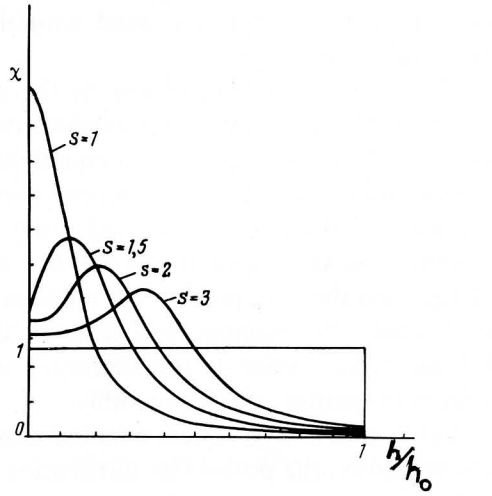


Fig. 5. The field dependence of the susceptibility for different values of $S \sim 1$.

the susceptibility is a monotonically decreasing function of the field. Starting from $S = 3/2$, the susceptibility increases for weak fields, and then passes through a maximum, which exists for arbitrarily large spin values. Since the existence of the maximum is a pure quantum effect, there is always a range of fields for which the classical treatment fails. If the spin is not small, then a typical change of the susceptibility occurs at field intensities close to critical (a rigorous criterium will be established below), in which essential differences between quantum mechanical and classical results are to be expected. In particular, the point $B = B_0$ itself is not singular for the quantum system. The results of perturbation theory have nothing to do with the field range $B \sim B_0$, which is most interesting from the physical viewpoint. As for characteristic equations of the type (2.23), although they allow one to perform numerical calculations for specific spin values, they are not convenient to investigate the analytical dependence of the quantities of interest to us on field and spin values. Therefore, to investigate the system for field intensities close to critical, the effective potential method is rather convenient and obvious.

This method appears to be especially useful for sufficiently high spin values. We emphasize that the condition $S \gg 1$ is quite realistic. First, it is realized in superparamagnets [Bean 1955; Bean and Livingston 1959]. On the other hand, as we shall see, the corresponding results, formally valid as $S \to \infty$, yield a rather good accuracy for $S \lesssim 10$, and they can therefore be applied to conventional paramagnets.

For spins $S \gg 1$ the typical behaviour of the magnetization (fig. 4) and susceptibility (figs. 5, 6) is caused by an essential restructuring of the energy spectrum in the field range $|B - B_0| \sim B_0 S^{-2/3}$ through the change of the effective potential from one form into another (see fig. 1). In such fields the behaviour of the potential (2.9) can be well fitted for the ground state and low-lying excited states by a power law approximation being an expansion of hyperbolic functions in powers of x near $x = 0$. Performing a scaling transformation of the coordinate $x = (S + \frac{1}{2})^{-1/3} q$, and confining ourselves to the main terms in $B - B_0$ in the expansion coefficients, we get the Hamiltonian corresponding to eq. (2.8),

$$H_{\text{eff}} = -B(S + \tfrac{1}{2}) + (S + \tfrac{1}{2})^{2/3}[p^2 + \tfrac{1}{4}q^4 + \gamma q^2 + \mathrm{O}(S^{-2/3})], \tag{2.26}$$

where $p = -\mathrm{i}\,\partial/\partial q$, and the parameter $\gamma = (S + \frac{1}{2})^{2/3}(B - B_0)/B_0$ is introduced, which in the most interesting physical range mentioned above takes the values $|\gamma| \sim 1$. In the vicinity of a critical magnetic field ($|\gamma| < 1$) the potential profile (2.9) is determined by the quartic term, and the quadratic term acts as a correction.

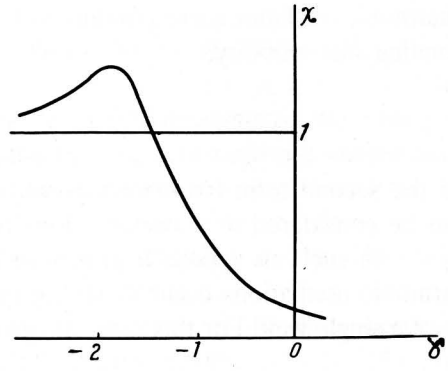


Fig. 6. The field dependence of the susceptibility for $S \gg 1$.

In the case of a critical magnetic field, when $\gamma = 0$, we get a purely quartic oscillator. The properties of such an oscillator have been studied in numerous papers (see, e.g., Chan and Stelman [1963], Chan et al. [1964]). The calculation yields the following results. The ground state energy is

$$E_0 = -2(S + \tfrac{1}{2})^2 + 0.668(S + \tfrac{1}{2})^{2/3}, \tag{2.27}$$

where the first term corresponds to the classical result for the potential minimum, and the second one is a quantum correction caused by the contribution of the zero-point oscillation energy. (Here and below, according to the expansion (2.26), we neglect the terms $\sim S^{-2/3}$ with respect to the last retained ones and present all the numerical results rounded off to three significant digits.) The magnetization equals

$$\langle S_x \rangle = S + \tfrac{1}{2} - 0.287(S + \tfrac{1}{2})^{1/3}. \tag{2.28}$$

As should be expected, it is not higher than the maximum admissible value S due to the negative term, compared to which the correction $1/2$ is small. Note that the dependence of the ground state energy and the corresponding magnetization on the spin value is not analytical. The susceptibility appears to be rather small, $\chi = 0.138$.

The correction quadratic in the coordinate in formula (2.8) is evaluated using perturbation theory (the quartic oscillator remains the unperturbed system). For fields with $\gamma < 0$, when the potential has the form of a well with two minima, it allows one to investigate the behaviour of the magnetic properties up to the "tangent" field ($\gamma = -0.881$), when the ground level coincides with the maximum of the barrier separating the wells. Then the energy is

$$E_0 = -2(S + \tfrac{1}{2})^2 + 1.76(S + \tfrac{1}{2})^{4/3},$$

the magnetization is

$$\langle S_x \rangle = S + \tfrac{1}{2} - 0.518(S + \tfrac{1}{2})^{1/3},$$

and the susceptibility is $\chi = 0.469$.

However, for lower magnetic field strengths ($\gamma < -1$) near the expected susceptibility maximum the zero-point oscillations essentially differ from the typical ones of the quartic oscillator. In the region of sufficiently small fields $B_0 - B \gg B_0 S^{-2/3}$ ($|\gamma| \gg 1$) another version of perturbation theory holds. The unperturbed system here is the harmonic oscillator corresponding to local oscillations in a single well. In the expressions for the corresponding susceptibility,

$$\chi \simeq 1 + B_0^2/(B_0^2 - B^2)^{3/2}, \tag{2.29}$$

unity is the classical result, and the second term is induced by zero-point oscillations. The effect of anharmonicity and tunneling can be considered as a perturbation. Nonetheless, in the region of the susceptibility maximum ($-3 < \gamma < -1$) such an approach proves to be too rough an approximation.

Note, by the way, that anharmonic oscillations occur in strong magnetic fields, $B - B_0 \gg B_0 S^{-2/3}$, when the potential has the form of a single well. For this case, the ground state susceptibility is a small quantity,

$$\chi \simeq \frac{B_0^2}{4[(B-B_0)B]^{3/2}}\,, \tag{2.30}$$

whereas, according to the classical concept, the susceptibility is strictly equal to zero, provided that $B > B_0$.

The above mentioned semiclassical approach precisely yields results of the type (2.29) and (2.30). Formal application of such expressions as $B \to B_0$ leads to divergences, which directly concern the contradictions mentioned. But actually, these formulae are valid only for fields far from critical. For fields close to critical, the terms omitted in the semiclassical approach from the Hamiltonian expansion in Bose operators become important. Since the semiclassical approach is general and applicable to arbitrary spin systems, it is interesting to dwell on this point and to analyse the causes of the arising contradictions using the same method.

Let us choose, following the semiclassic approach, the quantization axis x' along the classical equilibrium direction, and denote the angle between the x'-axis and the x-axis by θ. Taking advantage of the Holstein–Primakoff [1940] representation

$$\begin{aligned} S'_x &= S - a^+ a\,, \\ S'_+ &= S'_y + \mathrm{i}S'_z = \mathrm{i}\sqrt{2S - a^+ a}\, a\,, \\ S'_- &= S'_y - \mathrm{i}S'_z = -\mathrm{i}a^+\sqrt{2S - a^+ a}\,, \end{aligned} \tag{2.31}$$

where a^+ and a are creation and annihilation operators, let us expand the roots in a series. The equilibrium value of the angle can be found from the cancellation conditions for the terms linear in a and a^+ in the Hamiltonian: If $B < B_0$, there are two equilibrium positions, viz. $\theta = \pm\arccos(B/B_0)$, while for $B > B_0$, there is only one position $\theta = 0$. The corresponding oscillator frequency (in the system of units in which $\hbar = 1$) is $(B_0^2 - B^2)^{1/2}$ if $B < B_0$, and $[B(B-B_0)]^{1/2}$ if $B > B_0$. The corresponding expressions for the susceptibility are given by eqs. (2.29) and (2.30).

The divergence for $B \to B_0$ is caused by the fact that the approximation is too rough: It is the anharmonicity effect which turns out to be essential (even principal) for fields close to B_0, and the contribution of the anharmonicities should be considered together with the quadratic part of the Hamiltonian. In so doing, the magnetization oscillations cannot already be regarded as small. So, for fields weaker than B_0, or close enough to this value, the zero-point oscillation amplitude becomes comparable with the distance between both equilibrium values of θ, hence the choice of the quantization axis oriented along either of the corresponding directions is not justified. It is convenient here to choose the axis in a common manner for both $B > B_0$ and $B < B_0$ on the basis of symmetry arguments, directing it along the x axis. According to the above arguments, in the Hamiltonian expansion in a and a^+, one should retain the terms of both second and fourth order (there are no odd powers). Then the Hamiltonian takes the form

$$H = -B(S + \tfrac{1}{2}) + \tfrac{1}{2}(B - B_0)(a + a^+)^2 - \tfrac{1}{2}B(a - a^+)^2 + \tfrac{1}{8}[(a + a^+)(a^+ a^2 + a^{+2} a) + \text{h.c.}]\,. \tag{2.32}$$

Let us express the operators a and a^+ in terms of the dimensionless coordinates q in the following manner:

$$a = \frac{(S+\frac{1}{2})^{1/6} q + (S+\frac{1}{2})^{-1/6}\, \mathrm{d}/\mathrm{d}q}{\sqrt{2}}, \qquad a^{+} = \frac{(S+\frac{1}{2})^{1/6} q - (S+\frac{1}{2})^{-1/6}\, \mathrm{d}/\mathrm{d}q}{\sqrt{2}}. \tag{2.33}$$

Such a substitution allows one to single out in the operator part of the Hamiltonian a common factor dependent on the spin value, and to determine the field range in which the quartic terms should be taken into account. Actually, retaining the terms of first order in S^{-1}, we also get the Hamiltonian (2.27) derived above within the effective potential method.

Apparently, the expansion in powers of inverse spin based on eq. (2.31) results in a combined coordinate–momentum (owing to the terms of the type $\mathrm{d}/\mathrm{d}q$) Hamiltonian as an infinite series in powers of operators and momentum, whereas the effective potential method allows us from the very beginning to use rigorously the correspondence between the spin system and a particle moving in a potential field.

Let us return to a discussion of the properties of the spin system under consideration in the vicinity of the critical magnetic field on the basis of the Hamiltonian (2.26). Generally speaking, the oscillations here become essentially nonlinear owing to a rearrangement of the energy spectrum: Whereas for fields with $\gamma \gg 1$ the arrangement of the low-lying levels is approximately equidistant, in the vicinity of the critical field $|\gamma| \sim 1$ the arrangement corresponds to that of a quartic oscillator, and in the range $\gamma \lesssim -1$ the first excited level draws together with the ground state according to tunnelling splitting in a sufficiently deep well (spin tunnelling is discussed in detail in section 4).

In order to treat an "islet" of intermediate values of the magnetic field strength ($-3 < \gamma < -1$), where the susceptibility maximum is positioned, a quasiclassical approximation is applied with allowance for a peculiarity of the effective potential, in the form of a barrier between the wells (fig. 1a) [Ulyanov 1973; Zilberman 1957; Lifshitz and Kaganov 1962]. Using this approximation, one can obtain all the details of the susceptibility behaviour which are interesting for us in the magnetic field range $-3 < \gamma < -1$ including the vicinity of the maximum where the relative error even for the susceptibility does not exceed 2%.

The fact that, using quasiclassical methods and allowing for the peculiarity of the potential, one manages to reproduce fine details of the structure of the energy spectrum once more demonstrates the ample possibilities of the quasiclassical method even in a study of the ground state of the system [Ulyanov 1982].

For higher values of the magnetic field strength ($\gamma > -1$), where the energy of the ground level is higher than the maximum of the potential, high accuracy, as was stated above, is provided by perturbation theory on the basis of a quartic oscillator. The results of the quasiclassical approach and the ones of the perturbation theory match rather well.

Numerical methods were used to verify all the applied analytical approximations. The susceptibility appears to reach a maximum $\chi_{\max} = 1.31$ for a field strength corresponding to $\gamma = -1.87$. Then the energy gap between the ground and first excited states equals $\Delta E_0 = 0.141(S+\frac{1}{2})^{2/3}$.

To estimate the efficiency of the power law approximation relevant to the case $S \gg 1$, the results for the susceptibility presented in fig. 6 have been compared with the ones obtained numerically for $S = 10$. In the region of the susceptibility maximum the relative error does not exceed 10%. If the first omitted terms in expression (2.26) are taken into account, the relative error of the power law approximation decreases by an order of magnitude even for $S \sim 1$.

Let us stress that the results relevant to the power law approximation (2.26) for the effective potential are interesting by themselves since the quantum problem of a particle moving in such fields appears in widely different fields of quantum theory.

Note that the behaviour of the magnetization in the ground state with varying magnetic field essentially depends on the type of anisotropy, i.e., on the sign of α [see eq. (2.1)]. Thus, in the system considered with $\alpha > 0$ (recall that the condition $\alpha = 1$ was used in the corresponding formulae) the behaviour of the magnetization is continuous, whereas for $\alpha < 0$, in a field orthogonal to the "easy plane" and weaker than the corresponding critical field strength this behaviour is discontinuous [Filatova and Tsukernik 1969; Rosenfeld 1976]. This difference in quantum properties results in different roles of the low-temperature corrections: They are exponentially small in the former case, whereas in the latter they cause characteristic smoothing of the discontinuities of the magnetization.

Thus, as a result of a consistent quantum mechanical solution of the problem, it has turned out that in the vicinity of the critical magnetic field a sufficiently smooth change of magnetization occurs in the ground state for all spin values except $S = 1/2$ and $S = 1$ (see fig. 4, in which the dashed line corresponds to the classical broken behaviour). It has also turned out that the discontinuous behaviour of the classical susceptibility is altered to a smooth behaviour, the smoothing, however, being accompanied by the emergence of a maximum (fig. 5). Moreover, this maximum remains in the limit of arbitrarily large spin values (fig. 6) and emerges due to the rearrangement of the energy spectrum which occurs for $S \gg 1$ in the near-critical range of magnetic fields $|B - B_0| \sim B_0 S^{-2/3} \sim S^{1/3}$.

The investigation of all these fine effects has required the development and application of special methods. From this viewpoint, the effective potential method has proved to be especially obvious and efficient.

For high spin values ($S \gg 1$) in the indicated most important near-critical range of magnetic fields, the effective potential is fitted by a polynomial in the coordinates. The problem is thus reduced to the investigation of an essentially anharmonic oscillator in which the term of the fourth order in the coordinates plays the main role. We emphasize once more that at the critical magnetic field strength B_0 we get a purely quartic oscillator. For fields $|B - B_0| \ll S^{1/3}$ the second-order term serves as a correction, and perturbation theory works. In the field range $B_0 - B \lesssim S^{1/3}$, the motion of an effective particle is described by local oscillations in a single well, being caused by tunnelling (fig. 1a). A rather high precision here is provided by the quasiclassical approximation with allowance for the peculiarity of the potential in the form of a barrier separating the wells. This confirms once more the efficiency of quasiclassical methods even for the case of the ground state and a potential with peculiarities. Both approximations match well and reproduce all details of the behaviour of the magnetization and susceptibility.

In order to investigate in more detail the vicinity of the susceptibility maximum and to control the precision of the applied analytical methods, the effective stationary Schrödinger equation was numerically solved. The results obtained describe the behaviour of the considered spin system for sufficiently low temperatures for practically all values of the magnetic field and spin.

2.7. An effective potential for a many-particle system: the pseudospin Lipkin–Meshkov–Glick model

In the previous sections, an effective potential was constructed for a single-spin system. In this section we discuss an example of a many-particle (fermion) system whose energy spectrum can also be described with the effective potential method [Zaslavskii 1985]. This turns out to be possible by singling out a collective pseudospin degree of freedom of the system.

We shall deal with the model of Lipkin–Meshkov–Glick (LGM) used earlier [Lipkin et al. 1965] to verify different approximate methods in the theory of many particles (specifically, of a nucleus).

Interest in the LGM model increased recently in connection with studies of critical phenomena

[Gilmore and Feng 1978a, b; Feng et al. 1979; Gilmore 1981]. It was established that it describes a many-particle quantum mechanical system having classical properties. This is caused by the validity of the mean-field approximation [Gilmore 1981] as $N \to \infty$ (N being the number of nucleons) when this theory describes phase transitions in nuclear matter [Gilmore and Feng 1978a, b]. In this respect, it can be compared with the Dicke model [Dicke 1954], which describes the interaction of atoms with an electromagnetic field. The above mentioned approximation allows one to treat phase transitions in such systems on the general basis of catastrophe theory [Gilmore 1981].

The possibility of the above indicated potential description turns out to be one more interesting property of the LGM model. With its aid one can investigate the behaviour of the system in both the quantum and the classical regions in a common manner on the basis of the Schrödinger equation in which N^{-1} plays the role of the Planck constant. This method is especially convenient for $N \gg 1$; it gives the opportunity to investigate analytically the dependence of the ground state energy and the average number of particles (of excited nucleons) on the total particle number and the coupling constant, and to investigate smearing of the phase transition due to quantum fluctuations caused by the finiteness of N.

On the other hand, the rigorous description of collective effects using the single-particle Schrödinger equation has a certain interest by itself.

The LGM model Hamiltonian is

$$H = \tfrac{1}{2}\varepsilon \sum_{p,\sigma} \sigma a^{+}_{p,\sigma} a_{p,\sigma} + \frac{V}{2N} \sum_{p,p',\sigma} a^{+}_{p,\sigma} a^{+}_{p',\sigma} a_{p',-\sigma} a_{p,-\sigma} + \frac{W}{2N} \sum_{p,p',\sigma} a^{+}_{p,\sigma} a^{+}_{p',-\sigma} a_{p',\sigma} a_{p,-\sigma} , \tag{2.34}$$

where $a^{+}_{p,\sigma}$ and $a_{p,\sigma}$ are Fermi creation and annihilation operators, p varies from unity to N, V and W are the interaction parameters, $\sigma = \pm 1$, and $\varepsilon > 0$.

As follows from the Hamiltonian structure, the states with one fermion at fixed p (and different σ) form an invariant subspace. If one restricts oneself to this type of states [Lipkin et al. 1965], then such a model can be treated as a set of interacting two-level systems ("nucleons").

If there is no interaction, all ground state fermions are on the lowest level ($\sigma = -1$), and the elementary excitation energy is ε.

The space of states of the model has dimension 2^N. It turns out, however, that it can be divided into multiplets of essentially lower dimension owing to a certain symmetry of the system [Lipkin et al. 1965]. Specifically, if so-called pseudospin operators are introduced,

$$\begin{aligned} J_{+} &= \sum_{p} a^{+}_{p,(+)} a_{p,(-)} , \qquad J_{-} = \sum_{p} a^{+}_{p,(-)} a_{p,(+)} , \\ J_z &= \frac{1}{2} \sum_{p,\sigma} \sigma a^{+}_{p,\sigma} a_{p,\sigma} = n_{+} - \tfrac{1}{2}N , \qquad n_{+} = \sum_{p} a^{+}_{p,(+)} a_{p,(+)} , \end{aligned} \tag{2.35}$$

satisfying the commutation relations for momentum components, then the Hamiltonian (2.34) can be rewritten as follows:

$$H = \varepsilon J_z + \frac{V}{2N} (J^2_{+} + J^2_{-}) + \frac{W}{2N} (J_{+} J_{-} + J_{-} J_{+}) . \tag{2.36}$$

The operator $\boldsymbol{J}^2$ commutes with the Hamiltonian (2.34) so that the whole space of states is divided into subspaces with fixed J, each having dimension $2J + 1$. It obviously follows from eq. (2.35) that the maximum value of J is $N/2$.

We consider here the LGM model for $V = W = -g/2 < 0$ (the effective potential for a more general case will be discussed below in section 4 while considering tunnelling). (It should also be noted that Lipkin et al. [1965] investigated the model numerically for $W = 0$; Gilmore and Feng [1978b] used Bogolubov–Lieb inequalities describing the LGM system rather roughly.)

Now, the Hamiltonian can be cast into the form

$$H = -\varepsilon J_x - \frac{g}{N} J_z^2 \tag{2.37}$$

(a canonical transformation convenient for our further considerations was performed here: $J_x \to J_z$, $J_z \to -J_x$, $J_y \to J_y$).

Let us pay attention to the following analogy: For each fixed J the Hamiltonian (2.37) coincides up to notation with the Hamiltonian (2.1) describing a paramagnet with "easy-axis" anisotropy in a magnetic field orthogonal to this axis. Then the spin of the paramagnet equals J, the magnetic field is proportional to ε, the anisotropy constant is the coupling constant g, and the average number of excited nucleons (up to a constant) plays the role of the magnetization J_x (angular brackets indicate averaging over the ground state). This analogy allows us to take advantage of the methods and results of the preceding sections, in particular, those based on the paper by Zaslavskii et al. [1983], in which the properties of such a paramagnet were investigated.

In a purely classical approach (valid in the limit $N \to \infty$), neglecting the fact that different components J_i do not commute, we get the following result. The ground state corresponds to $J = N/2$, and for $g = \varepsilon$ a second-order phase transition occurs (the role of the order parameter being played by the average number of excited nucleons, nonzero for $g \geq \varepsilon$).

However, according to quantum mechanics, whatever $g \neq 0$ is, J_x cannot reach J since J_x has no definite value in a stationary state and, accordingly, $\langle n_+ \rangle \neq 0$ for $g \neq 0$. The system properties change smoothly (compare with the magnetization behaviour discussed in section 2.6).

In order to describe consistently the quantum mechanical properties of the system, let us introduce an effective potential in analogy with the procedure of section 2.6 to describe the properties of the paramagnet. The corresponding Schrödinger equation reads

$$\begin{aligned} &\frac{g}{N+1} \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + \left(\frac{E}{N+1} - U \right) \Psi = 0 , \\ &U = \frac{\varepsilon^2}{4g} \sinh^2 x - \frac{\varepsilon(J + \frac{1}{2})}{N+1} \cosh x \end{aligned} \tag{2.38}$$

(the substitution $g/N \to g/(N+1)$ was performed here).

Equation (2.38) makes apparent the physical meaning of the initial system for the coordinate system parameters. Specifically, the quantity $(N+1)^{-1}$ plays the role of Planck's constant (compare with Zaslavskii [1984b]), so that the statement on the asymptotic (in the limit $N \to \infty$) classical behaviour of the system under consideration gets an especially obvious meaning. As for the coupling constant g, it is analogous to the inverse mass. It is curious that, although the model contains the parameter ε related to the unperturbed system and the constant g describing the interaction between fermions and having the dimension of energy, the mass is determined exclusively by a coupling constant. In this respect one can say that the mass (to be more precise, the inverse mass) has a completely dynamical origin. The mass is the same for all multiplets.

The potential (2.38) is analogous to the one of eq. (2.9). The form of the effective potential can be essentially different depending on the coupling constant. If

$$g < g_0 = \varepsilon(N+1)/(2J+1)\,,$$

the potential represents a single well with a simple minimum (fig. 1c); it becomes a double well (fig. 1a) as $g > g_0$, and for $g = g_0$ a well with a fourfold minimum (fig. 1b) emerges.

The effective potential method allows one to find easily the multiplet corresponding to the ground state. As follows from eq. (2.38),

$$\frac{\partial E_0}{\partial J} = -\frac{\varepsilon}{N+1}\langle \cosh x \rangle < 0\,.$$

Therefore, for arbitrary N, the ground state lies in a multiplet with maximum possible $J = N/2$, $g_0 = \varepsilon$, and

$$U = \frac{\varepsilon^2}{4g}\sinh^2 x - \frac{\varepsilon}{2}\cosh x\,. \tag{2.39}$$

For low-lying states the potential U can be well approximated by a series expansion in the coordinate. It reduces to the anharmonic oscillator Hamiltonian, analogously to eq. (2.26). Quantum effects are essential for $|g-\varepsilon|/\varepsilon \sim N^{-2/3}$. In particular, when $g = \varepsilon$, the oscillator becomes purely quartic, and

$$\begin{aligned} &\langle n_+ \rangle = 0.228(N+1)^{1/3} - \tfrac{1}{2}\,, \\ &E_0/\varepsilon = -\tfrac{1}{2}(N+1) + 0.421(N+1)^{-1/3} \end{aligned} \tag{2.40}$$

(according to classical concepts, which neglect fluctuations, $\langle n_+ \rangle = 0$).

The first excited state also lies in a multiplet with $J = N/2$, the energy gap being $8.89 \times 10^{-2}(N+1)^{-1/3}\varepsilon$.

The analogy between the LGM model and single-particle systems is twofold. On the one hand, the collective behaviour of the fermions can be treated in terms of the magnetic characteristics of the relevant paramagnet, and on the other hand it is possible to describe it on the basis of the concept of quantum mechanical particle motion in an effective potential. Thus the present model serves as an example of the relationship between the energy spectra of three systems of an essentially different nature, viz., fermion, pseudospin, and coordinate systems. It is interesting that the model allows a clear description not only in the classical region, in which it undergoes changes typical for catastrophe theory [Gilmore 1981], but also in the quantum region due to the effective potential method.

This method allows one to define quite simply the multiplet in which the ground state lies and the width of the range near the phase transition where quantum effects related to the finiteness of the number of particles are essential, and also to calculate the ground state energy.

In conclusion of this section, let us emphasize once more that the effective potential method establishes relations between such seemingly different fields of theoretical and mathematical physics as the search for exact solutions of the Schrödinger equation and the analysis of cooperative effects.

3. Generalizations. Algebraic structure and physical meaning of quasi-exactly solvable models

In the preceding section we have considered a series of examples of potential models in which exact solutions could be found for only a finite number of low-lying states. Such systems were called quasi-exactly solvable [Turbiner 1988a, b]. The goal of this section is to analyse the algebraic and group-theoretical structure of the relevant Hamiltonian for the Schrödinger equation, to find a generalization of the above listed results, for which the Hamiltonian structure provides a basis, and to find relevant physical applications.

3.1. Potentials for biaxial paramagnets on the basis of spin coherent states

In section 2.1 the spin Hamiltonian corresponding to a uniaxial paramagnet has been analysed. Let us now investigate the case relevant to a single-particle spin system with a Hamiltonian of a more general quadratic–linear form describing (in application to magnetic phenomena) a biaxial paramagnet in an external magnetic field. Such a generalization can be done immediately for the spin Hamiltonian; however, within a coordinate picture it leads to qualitatively new results.

All the effective potentials turn out to be periodic, so that the exact solutions have a band nature. This is especially interesting because, although the quantum mechanical problem of a particle moving in a one-dimensional periodic potential is widespread in different fields of solid state physics, molecular vibrations, soliton theory, etc., the exact solutions (e.g. Kronig–Penney model, Dirac comb [Flügge 1971], and finite-band potentials [Zaharov et al. 1980]) are rare here, whereas models with simple explicit expressions for the energy band characteristics were found very recently [Zaharov et al. 1980; Razavy 1980, 1981; Zaslavskii and Ulyanov 1984, 1987].

In comparison with potentials corresponding to uniaxial anisotropy, considerably more cases with simple explicit solutions were found. Moreover, the new potentials are more different in form depending on the values of the entering parameters. For example, they can have simultaneously a fourfold minimum and a fourfold maximum.

As the parameters change, numerous interesting structural transformations take place, e.g., band coupling, emergence of new "spin" bands, and increase of the number of exact solutions.

The potentials found can be expressed in terms of elliptic functions. From them one can derive, by passing to different limits, a finite-band Lamé potential, which plays a significant role in the theory of solitons [Zaharov et al. 1980], as well as a series of other exactly solvable models known earlier (including aperiodic potentials, both localized and increasing at infinity), which have already been widely adopted. One can mention here the potentials of Morse, Eckart (specifically, the asymmetric one), Pöschl–Teller, as well as the spin potential of a uniaxial paramagnet. In this respect, the potentials found are generalizations combining in one picture those cases which seem to be so different. The relevant wave functions can be regarded as generalizations of the corresponding special functions.

The Hamiltonian of the spin system which describes the biaxial paramagnet in a magnetic field B orthogonal to the anisotropy axes can be written in terms of dimensionless quantities as follows:

$$H = \alpha S_z^2 - \beta S_y^2 + BS_x \,, \tag{3.1}$$

where $\alpha, \beta \geq 0$ are the anisotropy constants. The quadratic part of the Hamiltonian apparently corresponds to the most general structure of a Hermitian quadratic form (the case of non-Hermitian spin Hamiltonian will be discussed separately).

Let us demonstrate that the solution of the eigenvalue problem

$$H|\Psi\rangle = E|\Psi\rangle \tag{3.2}$$

for such a Hamiltonian leads to a second-order differential equation of the Schrödinger type with an effective potential. One of the options is a direct generalization of the approach developed in section 2.1, specifically, writing down the Schrödinger equation in the S_z representation, introducing a generating function, etc. Here we use another method being more consistent in bringing to light the algebraic nature of the relevant potential models. It is related to the representation of spin coherent states (SCS).

Following Radcliffe [1971] and Perelomov [1972, 1986], introduce nonnormalized SCSs according to the rule

$$|\xi\rangle = \mathrm{e}^{\xi S_-}|S\rangle = \sum_{\sigma=-S}^{S} \sqrt{\frac{(2S)!}{(S-\sigma)!(S+\sigma)!}}\, \xi^{S-\sigma}|\sigma\rangle\,, \tag{3.3}$$

where the complex parameter ξ characterizes the given SCS, $S_- = S_x - \mathrm{i}S_y$ is a lowering operator, the second equality in eq. (3.3) yields the expansion of the SCS in eigenvectors $|\sigma\rangle$ of the projections S_z. In Dirac notation an arbitrary state has the form

$$\Psi(\xi^*) = \langle \xi|\Psi\rangle = \sum_{\sigma=-S}^{S} \sqrt{\frac{(2S)!}{(S-\sigma)!(S+\sigma)!}}\, (\xi^*)^{S-\sigma}\langle\sigma|\psi\rangle = (\xi^*)^S \Phi\,. \tag{3.4}$$

Let us restrict ourselves to the unit circle in the plane of the complex parameter ξ, i.e., let us set $\xi = \mathrm{e}^{\mathrm{i}\varphi}$. Then, as follows from eq. (3.4),

$$\Phi(\varphi + 2\pi) = \mathrm{e}^{2\pi \mathrm{i} S}\Phi(\varphi)\,, \tag{3.5}$$

so that we get periodic functions for integer spins S, and antiperiodic functions for half-integer ones. Using the commutation relations for the spin projections S_j and eqs. (3.3) and (3.4) we come to the following explicit form of the action of the spin operator on the functions:

$$\tilde{S}_x = S\cos\varphi - \sin\varphi\,\frac{\mathrm{d}}{\mathrm{d}\varphi}\,,\quad \tilde{S}_y = S\sin\varphi + \cos\varphi\,\frac{\mathrm{d}}{\mathrm{d}\varphi}\,,\quad \tilde{S}_z = -\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}\varphi}\,. \tag{3.6}$$

Note that formulae (3.6) correspond, up to a similarity transformation, to the relevant relations for the generators of the spin representation of the rotation group listed by Naymark [1958]. They can also be immediately derived introducing a generating function constructed with the aid of conventional spin functions of the S_z representation, c_σ, according to the formula

$$\Phi(\varphi) = \sum_{\sigma=-S}^{S} \frac{c_\sigma}{\sqrt{(S-\sigma)!(S+\sigma)!}}\, \mathrm{e}^{\mathrm{i}\sigma\varphi}\,, \tag{3.7}$$

and taking into account the rules for the action of the spin operator in this representation. The relation to SCSs reveals the actual meaning of the spin–coordinate correspondence (in particular, of the φ-representation).

The desired differential form of eq. (3.2) for the eigenvectors and eigenvalues (EVA) of the spin Hamiltonian (3.1) under consideration can be obtained from the above defined rules for the transition to the φ-representation of SCSs. After substituting expressions (3.6) into the operators (3.1) and some not too complicated algebra eq. (3.2) becomes a second-order differential equation,

$$(\alpha + \beta\cos^2\varphi)\frac{d^2\Phi}{d\varphi^2} + [B\sin\varphi + \beta(S - \tfrac{1}{2})\sin 2\varphi]\frac{d\Phi}{d\varphi}$$

$$+ (E - BS\cos\varphi + \beta S^2\sin^2\varphi + \beta S\cos^2\varphi)\Phi = 0\,. \tag{3.8}$$

Intending to eliminate the first derivative, and to fix simultaneously the coefficient before the second derivative, we make the following substitution of variables:

$$\Psi = \Phi(\varphi)(\alpha + \beta\cos^2\varphi)^{-S/2}\exp\left(-\frac{B}{2\sqrt{\alpha\beta}}\operatorname{arctg}(\sqrt{\beta/\alpha}\cos\varphi)\right), \tag{3.9}$$

$$x = \sqrt{\alpha + \beta}\int_0^{\varphi}\frac{d\varphi'}{\sqrt{\alpha + \beta\cos^2\varphi'}} = F(\varphi, \sqrt{\beta/(\alpha + \beta)})\,, \tag{3.10}$$

where $F(\varphi, k)$ is an elliptic integral of the first kind with modulus k. Equation (3.7) is reduced to the normal form

$$(\alpha + \beta)\frac{d^2\Psi}{dx^2} + [E - U(x)]\Psi = 0\,. \tag{3.11}$$

Thus we come to the standard Schrödinger equation for a wave function (WF) Ψ in the coordinate x representation, which describes quasiparticle motion with a quadratic dispersion law [the inverse effective mass is $m^{-1} = 2(\alpha + \beta)$] in the effective potential

$$U(x) = \frac{[\frac{1}{4}B^2 - \alpha\beta S(S+1)]\,\mathrm{sn}^2 x + (\alpha + \beta)B(S + \frac{1}{2})\,\mathrm{cn}\,x}{\alpha + \beta\,\mathrm{cn}^2 x}\,, \tag{3.12}$$

composed of elliptic Jacobi functions [Abramowitz and Stegun 1964], the elliptic sine, $\mathrm{sn}\,x = \sin\varphi$, and elliptic cosine, $\mathrm{cn}\,x = \cos\varphi$. The potential is an even periodic function of x with period $4K$, where $K = K(k)$ is the complete elliptic integral of the first kind.

It should be noted that eq. (3.11) with the potential (3.12) is a generalization of a Lamé equation. This can be seen by replacing α and β in the equation by the modulus of the elliptic functions. However, we still use the form (3.11) and (3.12), which is more convenient from the application viewpoint, since the parameters α and β have a direct physical meaning. A discussion of passing to different limiting cases of already known exactly solvable models is contained in section 3.4.

Spin states correspond to solutions of eq. (3.11) of the type (3.9) satisfying the conditions

$$\Psi(x + 4K) = (-1)^{2S}\Psi(x)\,, \tag{3.13}$$

on the basis of eqs. (3.5), (3.9), and (3.10). It should be emphasized that eq. (3.11) with the conditions

(3.13) has, in addition to spin solutions, still other solutions (generally speaking, an infinite number). Since the wave functions (3.9) have, according to eq. (3.4), no more than $2S$ nodes, on the basis of the oscillation theorem for equations with a periodic potential [Kamke 1959] one can conclude that spin states correspond to numbers $n \leq 2S$. Since the symmetry group of the spin Hamiltonian is Abelian (the special case $B = 0$ will be discussed in section 3.3), and there is no degeneracy, then all energy levels of the spin system are the $2S + 1$ lowest energy levels of (anti)periodic states of the Schrödinger equation (3.11).

The obtained solutions allow a simple interpretation in terms of the band picture: They correspond to zero quasimomentum in the case of integer S, to quasimomentum equal to $\pi/4K$ in the case of half-integer S, and have to do with the alternating bottom and top of the energy bands. According to the general theory [Kamke 1959], periodic solutions can be described by wave functions with a number of zeros equal to 0, 2, 2, 4, 4, etc., and antiperiodic solutions by wave functions with the corresponding numbers equal to 1, 1, 3, 3, etc.

3.2. Properties of the effective potential and simple exact solutions

For fixed S the potential (3.12) is actually two-parametric, being dependent on B/α and β/α, whereas the potential corresponding to the unixial paramagnet in a transverse field (see section 2.1) is one-parametric. Moreover, in addition to the explicit dependence on β/α, there is also an implicit one arising from the modulus of the elliptic integral $k = \sqrt{\beta/(\alpha + \beta)}$. This results in wide variety of forms of the potential depending on the relation between B and typical critical values of the magnetic field,

$$B_{1,2} = \sqrt{S(S+1)(\alpha+\beta)^2 + \tfrac{1}{4}(\alpha-\beta)^2} \mp (S + \tfrac{1}{2})|\alpha - \beta| ,$$

and on that between α and β. As the magnetic field increases, there is a transition from a double minimum to a simple minimum via a fourfold one. As for the structure of the maximum of the effective potential, this changes in the reverse order, see fig. 7a ($\alpha < \beta$, $B = B_1$), fig. 7b ($B = B_0 = 2[\alpha\beta S(S + 1)]^{1/2}$), and fig. 7c ($B = B_2$). It is especially interesting that in the case $\alpha = \beta$ the potential can simultaneously have a fourfold maximum and a fourfold minimum at $B_0 = 2\alpha[S(S+1)]^{1/2}$ (fig. 8a).

Speaking about the structure of the energy spectrum, let us first draw the boundaries of its spin part. On the basis of the properties of the spin operators entering the Hamiltonian $H = \alpha S_z^2 - \beta S_y^2 + BS_x$ one can obtain the following simple inequalities for the energy level of the ground state:

$$-\beta S^2 - BS \leq E_0 \leq -\beta S^2 + \tfrac{1}{2}\alpha S ,$$

useful for $B \leq \beta(S - \frac{1}{2})$, and

$$-\beta S^2 - BS \leq E_0 \leq [\tfrac{1}{2}(\alpha - \beta) - B]S ,$$

for $B > \beta(S - \frac{1}{2})$. Analogous inequalities can also be derived for the energy level of the maximum spin state.

Such simple inequalities are significant for general qualitative estimates of the position of the whole energy spectrum and for a rough qualitative estimate of the energy level of the ground (or maximum spin) state as a function of the anisotropy parameters α and β and the magnetic field B.

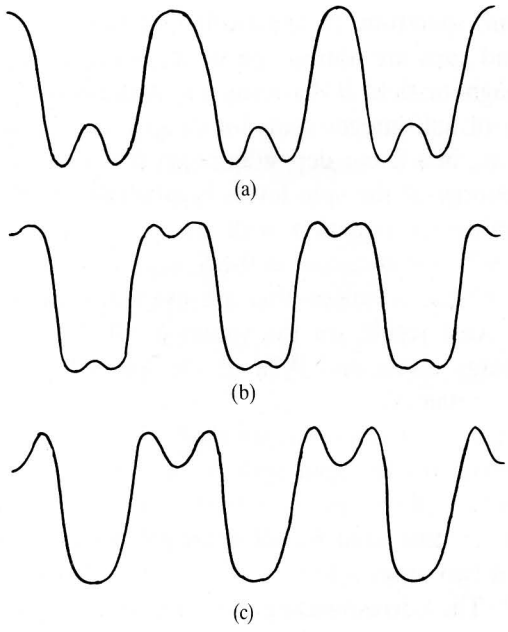


Fig. 7. The potential (3.12) for the biaxial case.

It is also essential that these inequalities yield a first approximation in the initial stage of the search for the energy levels in numerical calculations.

For large values of the magnetic field one gets for the Hamiltonian, using perturbation theory,

$$E_n = B(n - S) + (\alpha - \beta)[S(n + \tfrac{1}{2}) - \tfrac{1}{2}n^2] + \mathrm{O}(B^{-1}), \quad n = 0, 1, \ldots, 2S .$$

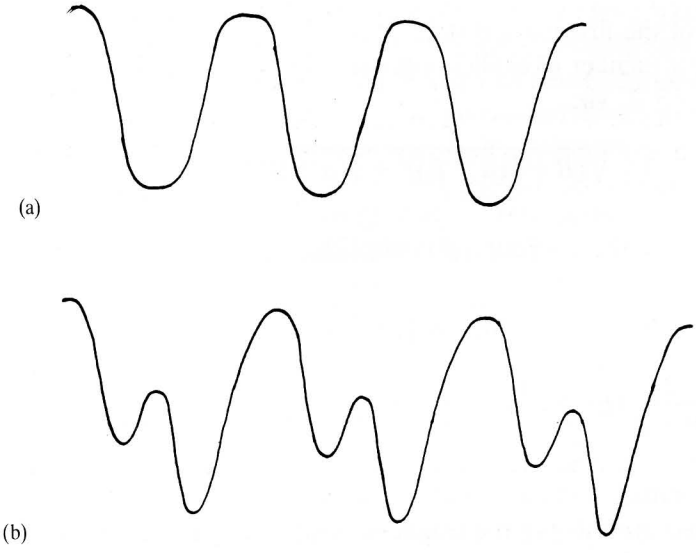


Fig. 8. (a) The potential (3.12) with a fourfold minimum and a fourfold maximum for $\alpha = \beta$, $B = 2\alpha[S(S+1)]^{1/2}$. (b) The potential (3.19) for the biaxial case for oblique magnetic field.

In the case $\alpha = \beta$ the spin spectrum is practically equidistant with level spacing $E_{n+1} - E_n = B + O(B^{-1})$, so that the band gaps are almost the same, being equal to B.

For small values of the magnetic field B the term BS_x in the Hamiltonian (3.1) can be regarded as a small correction. In the case of half-integer spins for doubly degenerate spin levels it results in a level splitting proportional to B, i.e., in a linear dependence on B of odd gaps in the spin bands. For integer spins the correction to the energy of the spin levels is quadratic in B.

With respect to the Schrödinger equation with the potential (3.12), the spin solutions can be regarded as exact since eq. (3.2), for instance, in the S_z representation can be reduced to a finite set of linear algebraic equations (with the solutions that are even in σ in eq. (3.2) separated from the odd ones, compare section 2.1). As a result, for the values $S = 0$, 1/2, 1, 3/2, and 2 one obtains simple explicit solutions for the energy levels and WFs of the spin states, whereby the relevant WFs and eigenvalues of eq. (3.11) are obtained.

Turning to a listing of simple exact solutions, we shall write for the WFs (3.9) only the factor $\Phi(\varphi)$. For the case $S = 0$ (being trivial for the spin system, but its potential undergoes changes of a form typical for the other S values as well) we get $E_0 = 0$, $\Phi_0 = 1$. Thus the bottom of the zeroth band for a periodic potential with $S = 0$ remains fixed for all deformations of the potential.

For $S = 1/2$ the energies of two exact solutions, $E_{0;1} = \frac{1}{4}(\alpha - \beta) \mp \frac{1}{2}B$, enclose the first gap between the bands, its width being B. The corresponding WFs are obtained by the expressions

$$\Phi_0 = \sin(\varphi/2)\,, \qquad \Phi_1 = \cos(\varphi/2)\,.$$

If $S = 1$, then

$$E_{0;2} = \tfrac{1}{2}(\alpha - \beta) \mp \sqrt{B^2 + \tfrac{1}{4}(\alpha + \beta)^2}\,, \qquad \Phi_{0;2} = \cos\varphi + \frac{E_{0;2} - \alpha}{B}\,,$$

$$E_1 = \alpha - \beta\,, \qquad \Phi_1 = \sin\varphi\,.$$

Curiously, the energy of the first excited state does not depend on B.

In general, the largest number of explicit solutions (for arbitrary values of the potential parameters) can be obtained for $S = 3/2$, viz.,

$$E_{0;2} = \tfrac{5}{4}(\alpha - \beta) - \tfrac{1}{2}B \mp \sqrt{(B + \tfrac{1}{2}(\alpha - \beta)]^2 + \tfrac{3}{4}(\alpha + \beta)^2}\,,$$

$$\Phi_{0;2} = \sin\tfrac{3}{2}\varphi + \frac{2}{B - \beta}\,(E_{0;2} - \tfrac{9}{4}\alpha + \tfrac{3}{4}\beta)\sin(\varphi/2)\,,$$

$$E_{1;3} = \tfrac{5}{4}(\alpha - \beta) + \tfrac{1}{2}B \mp \sqrt{[B - \tfrac{1}{2}(\alpha - \beta)]^2 + \tfrac{3}{4}(\alpha + \beta)^2}\,,$$

$$\Phi_{1;3} = \cos\tfrac{3}{2}\varphi + \frac{2}{B + \beta}\,(E_{1;3} - \tfrac{9}{4}\alpha + \tfrac{3}{4}\beta)\cos(\varphi/2)\,.$$

A new phenomenon (compare section 2.6) arises for the spin system (for $\alpha \neq \beta$), namely, the existence of a minimum of the absolute value of the magnetic susceptibility in either the ground and second states (if $\alpha < \beta$) or in the first and third ones (if $\alpha > \beta$).

In the general case with $S = 2$ (other possibilities are discussed below) simple exact solutions can be

obtained for the first and third excited states,

$$E_{1;3} = \tfrac{5}{2}(\alpha - \beta) \mp \sqrt{B^2 + \tfrac{9}{4}(\alpha + \beta)^2}\,,$$

$$\Phi_{1;3} = \sin 2\varphi - \frac{2}{B}\left[\tfrac{3}{2}(\alpha + \beta) \pm \sqrt{B^2 + \tfrac{9}{4}(\alpha + \beta)^2}\right]\sin\varphi\,.$$

For larger values of s, in general, the roots of the relevant characteristic equation cannot be found explicitly. However, one can obtain simple recursion relations for a polynomial, which define the characteristic equation with the aid of a continued fraction method giving an efficient computational algorithm for the energy levels. The most convenient representation in this case turns out not to be the S_z but the S_x representation resulting in three-term recursion relations for the spin wave functions c_σ,

$$(\alpha + \beta)[\sqrt{(S - \sigma)(S - \sigma - 1)(S + \sigma + 1)(S + \sigma + 2)}c_{\sigma+2}$$
$$+ \sqrt{(S + \sigma)(S + \sigma - 1)(S - \sigma + 1)(S - \sigma + 2)}c_{\sigma-2}]$$
$$- [E - B\sigma + \tfrac{1}{2}(\alpha - \beta)(\sigma^2 - S^2 - S)]c_\sigma = 0\,, \quad c_\sigma = 0, \forall|\sigma| > S\,.$$

Consider now a special range of parameters corresponding to a higher degree of symmetry of the system. The energy spectrum and the form of the potential have a series of interesting properties, while, on the other hand, the number of simple explicit solutions considerably increases.

3.3. Symmetry properties and additional exact solutions

In general, the symmetry group of the Hamiltonian (3.1) includes (in addition to the identity) a rotation by the angle π around the S_x-axis. The group is Abelian, so that the spin energy levels are not degenerate. Reversing the sign of the magnetic field B in the Hamiltonian (3.1) results in an equivalent Hamiltonian with the same energy spectrum. In a coordinate description this transformation corresponds to a shift of the origin of coordinates by half a period, $2K$. Analogously, the substitution $\alpha \leftrightarrow \beta$ in the Hamiltonian (3.1) results, with allowance for the above mentioned property, in an equivalent Hamiltonian of opposite sign, so that the spin system after such a substitution is reversed with respect to zero.

If $\alpha = \beta$, then the energy levels appear in pairs (E and $-E$). In particular, there is a level $E = 0$ for arbitrary B in the case of integer spin. For instance, if $S = 2$ and the levels are even (the odd ones were found in section 2.2), we get (for simplicity, we set $\alpha = \beta = 1$ in this section)

$$E_{0;4} = \mp 2\sqrt{B^2 + 3}\,, \qquad \Phi_{0;4} = \cos 2\varphi + \frac{8B}{E + 6}\cos\varphi + \frac{3(E - 2)}{E + 6}\,,$$

$$E_2 = 0\,, \qquad \Phi_2 = \cos 2\varphi - \frac{4}{B}\cos\varphi - 1\,.$$

If $S = 3$, then

$$E_{0;2} = -E_{6;4} = -\sqrt{5B^2 + 33 \pm 4\sqrt{B^4 + 6B^2 + 54}}\,, \qquad E_3 = 0\,, \qquad E_{1;5} = \mp 2\sqrt{B^2 + 15}\,.$$

The expressions for the wave functions for $S \geq 3$ are not presented here because they are rather cumbersome.

Nonzero levels for $S = 4$ can be written in compact form,

$$E_{\text{even}} = \mp\sqrt{10B^2 + 118 \pm 6\sqrt{B^4 - 2B^2 + 225}},$$

$$E_{\text{odd}} = \mp\sqrt{5B^2 + 113 \pm 4\sqrt{B^4 + 38B^2 + 550}}.$$

If $S = 5$, the analogous result for odd states reads

$$E = \mp\sqrt{10B^2 + 318 \pm 6\sqrt{B^4 + 38B^2 + 1225}}.$$

Now let $B = 0$. In this limiting case a new symmetry feature arises: For arbitrary α and β the Hamiltonian (3.1) becomes invariant under rotation by the angle π not only about the S_x-axis, but also about S_y (S_z). If the spin is half-integer, such transformations anticommute with each other resulting in a degeneracy of the energy levels (in the case of integer spin the symmetry group remains Abelian and degeneracy does not arise).

As a result, for $\alpha = \beta$ and $B = 0$ one can find explicit expressions for the characteristics of states with higher values of S,

$$S = 5/2: \quad E_{0;1} = -E_{4;5} = -2\sqrt{7}, \qquad E_{2;3} = 0,$$

$$S = 7/2: \quad E_{0;1} = -E_{6;7} = -\sqrt{63 + 12\sqrt{21}},$$

$$E_{2;3} = -E_{4;5} = -\sqrt{63 - 12\sqrt{21}},$$

$$S = 9/2: \quad E_{0;1} = -E_{8;9} = -\sqrt{198 + 6\sqrt{561}},$$

$$E_{2;3} = -E_{6;7} = -\sqrt{198 - 6\sqrt{561}},$$

$$E_{4;5} = 0.$$

We present here the formula for $\Phi(\varphi)$ for the simplest case $S = 5/2$ in the ground state,

$$\Phi_0 = \sin\tfrac{5}{2}\varphi - \tfrac{1}{3}(11 + 4\sqrt{7})\sin\tfrac{3}{2}\varphi - 2(5 + 2\sqrt{7})\sin\tfrac{1}{2}\varphi. \tag{3.14}$$

Regarding the symmetry properties of the potential $U(x)$, it should be stressed that for $B = 0$ the potential period decreases by a factor of two; hence the period in quasimomentum space doubles. As a result, pairwise merging of bands occurs and all odd gaps disappear. Moreover, for integer S the spin energy levels correspond to the edges of all the merged bands. In addition, in this case the system has the interesting property of finite bands (see section 3.4). If S is half-integer, the energy levels corresponding to the quasimomentum values $\pi/4K$ and bordering odd gaps turn out to be degenerate (whether they are spin bands or not).

In contrast, for $B \neq 0$ the period doubles and the superlattice effect of band splitting occurs. Such transformations of the bands can be called "magnetic" structure transitions.

As was pointed out above, in each of the lowest $2S+1$ bands for the effective potential (2.20) and (3.12), one of the last energy levels is a spin level; this allows one to call these bands spin bands. However, special attention is due to the higher, overspin bands. Their arrangement seems to have many features of interest.

Using numerical methods (with exact solutions serving as test examples), the following results were established [Ulyanov, unpublished]. If the parameter S varies continuously, then for each integer value S the even overspin gaps disappear, and for each odd S the odd ones do. This band pairing is accompanied by parity exchange between energy levels which border disappearing gaps, and also by transformation of the next overspin band to a spin band with emerging exact solutions. Thus we deal with periodic "spin" structure transitions. Pairing concerns all overspin bands, not a certain separate pair (vertical periodicity rule in the scheme of stability zones) and occurs at each integer or half-integer value of the potential spin parameter (horizontal periodicity rule).

It should be stressed that, in contrast to "magnetic" structure transitions, these transitions are not caused by any explicit symmetry of the potential; they concern only overspin bands. A rigorous mathematical proof and the discovery of the corresponding hidden symmetry are of interest. One can say that for the case of integer S band pairing is a consequence of the finiteness of the band: for $B \neq 0$, owing to the superlattice effect, all odd gaps open up, but even overspin gaps remain closed. For half-integer S the superlattice effect manifests itself only in spin bands, overspin bands remaining paired.

Notice that on the level with two critical parameter values (see section 3.2), there is yet another typical intermediate value $B_0 = 2[\alpha\beta S(S+1)]^{1/2}$ at which the potential becomes antiperiodic, specifically, $U(x+2K) = -U(x)$. Complete symmetry of barrier and well arises. (If $\alpha = \beta$, then all three base points B merge.)

3.4. Finite band and other limiting cases of elliptic potentials. Analogues based on SU(1, 1)

One of the interesting properties of the potentials found in this work is that these potentials comprise, in limiting cases, a series of well-known exactly solvable models which are widely used in physical applications, and that they are a generalization of them. For convenience, divide eq. (3.11) by $\alpha+\beta$ and express the coefficients of the potential $V = U/(\alpha+\beta)$ in terms of the moduli of the elliptic functions k and $k' = (1-k^2)^{1/2}$. Then

$$V = [\tfrac{1}{4}\mu^2 - k^2k'^2S(S+1)]\,\frac{\mathrm{sn}^2x}{\mathrm{dn}^2x} + \mu(S+\tfrac{1}{2})\,\frac{\mathrm{cn}\,x}{\mathrm{dn}^2x}\,, \quad \mu = \frac{B}{\alpha+\beta}\,. \tag{3.15}$$

The relevant spin Hamiltonian is

$$H = k'^2S_z^2 - k^2S_y^2 + \mu S_x.$$

We confine ourselves to transformations of the potential and the spectrum, omitting, for brevity, the issue of wave function behaviour.

As follows from the properties of elliptic functions [Abramowitz and Stegun 1964], for $k=0$ the potential changes to

$$V = \tfrac{1}{4}\mu^2 \sin^2 x + \mu(S+\tfrac{1}{2})\cos x\,,$$

whereas for $k = 1$ (and $\mu \to -\mu$) it changes to

$$V = \tfrac{1}{4}\mu^2 \sinh^2 x - \mu(S + \tfrac{1}{2}) \cosh x ,$$

i.e., to the potentials considered in section 2.

Make now the substitution of variable $x = u - K$ and renormalize the magnetic field $B = b(\alpha + \beta)k'$. Then the potential (3.15) becomes

$$V = [\tfrac{1}{4}b^2 - k^2 S(S+1)] \operatorname{cn}^2 u + b(S + \tfrac{1}{2}) \operatorname{sn} u \operatorname{dn} u , \tag{3.16}$$

and

$$H = k'^2 S_z^2 - k^2 S_y^2 + bk' S_x$$

(dn u being an elliptic function).

This form of the potential is most convenient since it immediately yields the Lamé equation in zero magnetic field ($b = 0$). If S is integer, then the Lamé potential has the important property of finiteness of the band [Bateman and Erdélyi 1955; Zaharov et al. 1980], and only S spin gaps remain, all higher gaps having disappeared. Such a potential refers to a certain particular case of periodic solutions of the Korteweg–De Vries equation. For instance, $S = 1$ refers to the one-gap Lamé potential which does not change with evolution (an analogue of a one-soliton solution).

If $k = 0$, then eq. (3.16) yields (for arbitrary S) a periodic potential

$$V = \tfrac{1}{4}b^2 \cos^2 u + b(S + \tfrac{1}{2}) \sin u .$$

For $k = 1$, we come to the generalized Eckart potential

$$V = \frac{\frac{1}{4}b^2 - S(S+1)}{\cosh^2 u} + \frac{b(S + \frac{1}{2}) \sinh u}{\cosh^2 u} .$$

In this case $H = -S_y^2$, and the discrete energy levels are $E_n = -(S - n)^2$ ($n_{\max} = S - 1$ for integer S and $n_{\max} = S - \frac{1}{2}$ for half-integer S).

Here and above x is regarded as real. But the substitution $x = i\eta$ results in a potential analogous to eq. (3.15) with the only difference that the moduli k and k' go over into each other. The sign and numbering of the spin energy levels are reversed (see section 3.3).

The above considered potentials are related to representations of the SU(2) algebra. Analogously, one can construct potentials on the basis of the SU(1, 1) algebra. If one proceeds from the generators K_0, K_1, K_2 [$K_0^2 - K_1^2 - K_2^2 = q(q-1)$, q being a group index] in the representation of relevant generalized coherent states [Perelomov 1986], then the Hamiltonian

$$H = k'^2 K_0^2 + k^2 K_1^2 + \lambda k k' K_2$$

can be shown to correspond to an effective potential

$$V = \frac{q(q-1) + \frac{1}{4}\lambda^2}{\operatorname{sn}^2 \eta} - \frac{\lambda(q - \frac{1}{2}) \operatorname{cn} \eta}{\operatorname{sn}^2 \eta} - k^2[\tfrac{1}{4}\lambda^2 + q(q-1)] . \tag{3.17}$$

In the limiting case $k = 0$, it changes to a generalized Pöschl–Teller potential

$$V = \frac{q(q-1) + \frac{1}{4}\lambda^2}{\sin^2\eta} - \frac{\lambda(q-\frac{1}{2})\cos\eta}{\sin^2\eta},$$

and for $k = 1$ to

$$V = \frac{q(q-1) + \frac{1}{4}\lambda^2}{\sinh^2\eta} - \frac{\lambda(q-\frac{1}{2})\cosh\eta}{\sinh^2\eta}.$$

Since here $H = K_1^2$, it is easy to pass to the limit of a continuous spectrum.

Let us make a few remarks on the spectra of two different group Hamiltonians, specifically, of SU(2) and SU(1, 1), in the simplest case of $B = 0$. If $q = S + 1$ is integer, then one gets a Lamé equation with a finite-band potential, with the low-lying energy levels (which define the gap positions) being spin levels by their origin. As for SU(1, 1), the overspin levels refer to it (being doubly degenerate according to disappearing forbidden bands). Thus two essentially different sets of energy levels of one and the same equation with periodic boundary conditions are described by different group Hamiltonians.

It should also be noted that, analogously to the potentials of spin nature, the substitution $\eta = i\xi$ results in a potential of SU(1, 1) type, which differs from eq. (3.17) by the substitution $k \leftrightarrow k'$.

Thus, from a common viewpoint, summarizing the results and using the complex x-plane, we come to the following conclusions. The real and imaginary axes refer to the effective spin potentials, each version comprising, as limiting cases, both the potential well and the periodic potential considered in section 2 (for a uniaxial paramagnet, we get only the potential well along the real axis and the periodic potential along the imaginary one). In addition, a generalized Eckart potential arises. Remember also that in the limit of small magnetic field the spin potential of the uniaxial paramagnet changes into the Morse potential (more precisely, to a superposition of two separate Morse wells, see section 2.3). As for periodic potentials connected with representations of the SU(1, 1) algebra, a variation of x corresponds to their being shifted along straight lines from the real or imaginary axes by K or K', respectively.

Notice that yet another algebraic approach based on the representations of SU(2) and SU(1, 1), which allows one to describe the properties of Morse and Eckart potentials, was developed by Alhassid et al. [1983] using a Schwinger representation. The relationship between the Lamé equation and the spin Hamiltonian was discussed earlier [Patera and Winternitz 1973; Miller 1977; Alhassid et al. 1983; Turbiner 1989]. In all these cases the spin Hamiltonian includes only terms quadratic in the group generators; this implies, from a physical point of view, that only anisotropy is taken into account (if one considers a paramagnet). Inclusion of the magnetic field described by a linear term and the use of generalized coherent states allow one to considerably increase the number of exact solutions and to obtain effective potentials with much more varied properties.

Notice the following directions of generalization of the obtained results. One of them is related to the consideration of spin systems which describe a biaxial paramagnet in a magnetic field with an arbitrary orientation. In particular, if the magnetic field lies in the plane containing one of the anisotropy axes, then the spin Hamiltonian takes the form

$$H = \alpha S_z^2 - \beta S_y^2 + BS_x + CS_y. \tag{3.18}$$

Following the arguments of section 3.1 step by step, we come to the corresponding result. The effective potential of the Schrödinger equation (3.11),

$$U(x) = [\tfrac{1}{2}(B\,\mathrm{sn}\,x - C\,\mathrm{cn}\,x)^2 - \alpha\beta S(S+1)\,\mathrm{sn}^2 x + (\alpha+\beta)B(S+\tfrac{1}{2})\,\mathrm{cn}\,x + \alpha(S+\tfrac{1}{2})C\,\mathrm{sn}\,x]/(\alpha+\beta\,\mathrm{cn}^2 x)\,, \tag{3.19}$$

becomes even more flexible through the new parameter C, being characterized by many asymmetric profiles, one of which is presented in fig. 8b as an example.

The wave functions of the stationary states $\Psi(x)$ are related to the functions of the SCS representation Φ via the formula

$$\Psi_n(x) = \Phi_n(x)\left(\frac{\sqrt{\alpha+\beta} - \sqrt{\beta}\,\mathrm{sn}\,x}{\sqrt{\alpha+\beta} + \sqrt{\beta}\,\mathrm{sn}\,x}\right)^{C/4\sqrt{\beta(\alpha+\beta)}} \times \frac{\exp[-(B/2\sqrt{\alpha\beta})\,\mathrm{arctg}(\sqrt{\beta/\alpha}\,\mathrm{cn}\,x)]}{(\alpha+\beta\,\mathrm{cn}^2 x)^{S/2}}\,. \tag{3.20}$$

All the above arguments on the relation between spin and band solutions hold in this case. However, there are fewer of them for which simple exact analytical expressions for the energy levels can be found.

For $S = 0$ the only spin energy level which determines the bottom of the lowest band remains zero, $E_0 = 0$, whereas $\Phi_0 = 1$ in eq. (3.20). For $S = 1/2$ the energy levels of the ground and first excited states,

$$E_{0;1} = \tfrac{1}{4}(\alpha - \beta) \mp \tfrac{1}{2}\sqrt{B^2 + C^2}\,,$$

enclose the first gap in the band spectrum of the potential (3.19), and

$$\Phi_0 = \sin\tfrac{1}{2}(\varphi - \varphi_0)\,, \qquad \Phi_1 = \cos\tfrac{1}{2}(\varphi - \varphi_0)\,, \quad \varphi_0 = \mathrm{arctg}(C/B)\,.$$

Different limits for the potential (3.19) can be considered in analogy with the previous section. In particular, one can thus obtain the asymmetric two-parametric (for fixed S) potentials already considered in section 2.4.

Analogously, one can consider a Hermitian quadratic–linear spin Hamiltonian of the general form

$$H = \alpha S_z^2 - \beta S_y^2 + BS_x + CS_y + DS_z\,.$$

A complex potential corresponds to it.

A further generalization lies in the consideration of quadratic–linear forms in terms of the components of spin operators of the most general form [Turbiner 1988c]

$$H = \sum_{\substack{i,j=+,0,-,\\ j\geq i}} a_{ij}S_iS_j + \sum_{i=+,0,-} b_iS_i\,, \tag{3.21}$$

without confining ourselves to Hamiltonians which are Hermitian in spin space. If one takes advantage of the representation for spin operators

$$S_+ = \partial/\partial z\,, \quad S_- = 2Sz + z^2\,\partial/\partial z\,, \quad S_0 = S_z = S - z\,\partial/\partial z \tag{3.22}$$

(which, in the particular case $z = e^{-i\varphi}$, can be reduced to eq. (3.6) after a similarity transformation), then for the generating function

$$\Phi = \sum_{\sigma=-S}^{S} \frac{c_\sigma}{\sqrt{(S-\sigma)!(S+\sigma)!}}\, z^\sigma \tag{3.23}$$

one gets a differential equation which can be written in the form

$$-P_4(z)\,\frac{d^2\Phi}{dz^2} + P_3(z)\,\frac{d\Phi}{dz} + [P_2(z) - E]\Phi = 0\,, \tag{3.24}$$

where $P_i(z)$ is a polynomial of ith order in z. If a_{ij} and b_i are real numbers, then these polynomials are real for real z. Proceeding in a similar manner as above, eq. (3.24) can be reduced to a Schrödinger equation of conventional form with an effective potential which generally can be expressed in terms of elliptic functions in a rather cumbersome way.

The correspondence between coordinate and finite-dimensional systems can be considered from yet another standpoint. Let us try, without introducing spin operators from the very beginning, to figure out which finite-difference equations are valid for the construction of effective potentials. Consider matrices of the simplest structure, i.e., three-diagonal ones, and the difference equation they refer to,

$$(w_\sigma - E)a_\sigma + p_\sigma a_{\sigma-1} + r_{\sigma+1}a_{\sigma+1} = 0\,. \tag{3.25}$$

Intending to obtain a second-order differential equation (after introducing the generating function), we restrict ourselves to coefficients which are real polynomials of second order in σ (similar to the consideration of forms quadratic in the generators in the method of the spin Hamiltonian). We are interested in cases in which the series in the generating function

$$\Phi = \sum_\sigma a_\sigma z^\sigma \tag{3.26}$$

is cut off so that the discrete variable σ lies in a finite range. Since one can, without any loss of generality, count from the mean value, let us set $-S \le \sigma \le S$, where $S \ge 0$ is an integer or half-integer. Finite-dimensional solutions of eq. (3.25) are possible, provided that the conditions

$$r_{-S} = p_{S+1} = 0 \tag{3.27}$$

hold. The coefficients a_σ entering the generating function Φ are related to the spin wave function in the S_z representation through the relationship

$$a_\sigma = c_\sigma/\sqrt{(S-\sigma)!(S+\sigma)!}\,.$$

The method of finite-dimensional matrices (including a discussion of the most general five-diagonal case) and the way it is used to derive potentials for which exact solutions exist for a part of the energy spectrum, have been considered in more detail by Zaslavskii [1990a].

3.5. *Effective potentials for systems with spin–boson and spin–spin interactions*

In general, the potential corresponding to the equation for the generating function (3.24) looks immense. However, there are a few particular cases for which it takes rather a simple form, being expressed in terms of elementary functions or simple combinations of elliptic functions. A series of such examples has already been considered in preceding sections. Another set of similar effective potentials have been found by Turbiner [1988a, b]. It is especially interesting that they correspond to an anharmonic oscillator (with a sextic anharmonicity), provided that certain relations hold between the coefficients of different powers of the coordinate.

Such potentials, as we shall see, refer to special cases of equations of the type (3.24) when the coefficient before the highest derivative (in general, a polynomial of the fourth or third order for three-diagonal matrices) either degenerates into a polynomial of lower order or has multiple roots, with the corresponding difference equation having a three-dimensional form. (In the papers by Turbiner [1988a, b, c] these potentials were derived in a different manner.)

An important issue is the physical interpretation of the potentials thus obtained. As we have already seen, such potentials may have an immediate physical meaning determined by the structure of the spin Hamiltonians these potentials are based on. These are, for instance, the effective potentials for uniaxial and biaxial (super) paramagnets. However, such an interpretation is clear only when the corresponding spin Hamiltonian is Hermitian in spin space, but this condition does not hold in general (see the end of the preceding section). Therefore, the physical meaning of such potentials is not apparent. Nevertheless, we are going to demonstrate that it does exist [Zaslavskii 1990d]. It turns out that these potentials describe systems with an interaction, including such well-known physical models as the Dicke model and the Heisenberg model (for two spins etc.) Let us turn to the consideration of specific examples.

Consider first the simplest model with a spin–boson interaction described by the Hamiltonian

$$H = \omega a^{+}a + \varepsilon S_z - g(a^{+}S_{-} + aS_{+}) . \tag{3.28}$$

Here a^{+} and a are Bose operators. Such a Hamiltonian is equivalent to the Dicke model [Dicke 1954] in a subspace with a fixed value of the angular momentum. There is an integral of the motion for the system,

$$R = S + S_z + a^{+}a , \tag{3.29}$$

which allows one to divide the whole infinite-dimensional space of states of the model into finite-dimensional subspaces with a fixed R value. For each multiplet the Schrödinger equation has the form

$$[E - \omega R + n(\omega - \varepsilon)]c_n + g[\sqrt{(n+1)(2S-n)(R-n)}\, c_{n+1} + \sqrt{n(2S+1-n)(R+1-n)}\, c_{n-1}] = 0 , \quad n = \sigma + S = 0, 1, \ldots, 2S , \tag{3.30}$$

where σ is the value of S_z. The substitution

$$c_n = b_n \sqrt{(R-n)!\, n!\, (2S-n)!} \tag{3.31}$$

results in the rationalized expression

$$[(\omega - \varepsilon)n + E - \omega R]b_n + g(n+1)b_{n+1} + g(2S+1-n)(R+1-n)b_{n-1} = 0 . \tag{3.32}$$

Introducing the generating function

$$\Phi = \sum_{n=0}^{2S'} b_n z^n , \quad S' = \min(S, R/2) , \tag{3.33}$$

one can get a differential equation for Φ. A similar method was used in an analysis of the Dicke model by Scharf [1974, 1975]. However, the equation derived there contains a variable coefficient; in this respect it is not a Schrödinger equation (it is more likely to correspond to an equation of the type (3.24) with respect to its structure). We reduce it to the form of a Schrödinger equation by the substitution

$$z = r^{-2} ,$$

$$\Psi = \Phi r^{R+2S+1/2} \exp(-\tfrac{1}{4}r^4 + \tfrac{1}{2}\mu r^2) , \tag{3.34}$$

$$\mu = (\varepsilon - \omega)/g .$$

As a result, we get

$$\mathrm{d}^2\Psi/\mathrm{d}r^2 + (\kappa - U)\Psi = 0 , \tag{3.35}$$

$$U = r^6 - 2\mu r^4 + (\mu^2 - 2R - 4S - 4)r^2 + [(R-2S)^2 - \tfrac{1}{4}]r^{-2} + 2\mu(R + 2S + 1) , \tag{3.36}$$

$$\kappa = (4/g)(E + \varepsilon S - \omega R) .$$

The structure of the wave function (3.33), (3.34) exhibits a rapid decrease of Ψ at infinity and its behaviour in the limit $r \to 0$ is $\Psi \sim r^{|R-2S|+1/2}$.

The potential (3.36), which corresponds to the anharmonic oscillator with a centrifugal barrier, was derived by Turbiner [1988a] from other arguments.

Let us next consider the more complicated Hamiltonian

$$H = -\alpha S_z^2 + BS_z + \omega a^+ a - g(a^+ S_- + aS_+) . \tag{3.37}$$

It can describe, for instance, a spin–phonon interaction. Here α plays the role of the constant of anisotropy induced, for instance, by a crystal field [White 1983]. B is a magnetic field, up to a factor. Just as in the previous case, the integral of the motion (3.29) divides the whole space into multiplets with different R. For each multiplet we have a Schrödinger equation (3.35) with eigenvalue

$$\kappa = (4/\alpha)(E + \alpha S^2 + BS - \omega R) ,$$

and potential (up to a factor)

$$
\begin{aligned}
&U = C_1 \sinh^{-2}x + C_2 \cosh^{-2}x + C_3 \cosh^2 x + C_4 \cosh^4 x\,,\\
&C_1 = (R-2S)^2 - \tfrac{1}{4}\,,\\
&C_2 = -(R+2S)^2 + 2(R+2S)(\tau^2 + \mu\tau - 1) - \tfrac{3}{4} - \tau^4 + \tau^2(2-\mu^2) + 2\mu\tau(1-\tau^2)\,,\\
&C_3 = -2\tau^2(1 + \mu\tau + \tfrac{3}{2}\tau^2)\,,\\
&C_4 = \tau^4\,,\\
&\tau = g/\alpha\,, \quad \mu = (B - \omega + 2\alpha S)/g\,.
\end{aligned}
\tag{3.38}
$$

The coordinate transformation which relates x and z has the form

$$
z = (\alpha/g)\sinh^{-2}x\,. \tag{3.39}
$$

The generating function is analogous to the one of eq. (3.33).

The relation between eqs. (3.35) and (3.38) is not apparent; however, in the limiting case $\alpha \to 0$ the coordinate transformation formulae are $z \sim (\alpha/g)x^{-2}$, $x \sim r\sqrt{\alpha/g}$, and a direct computation confirms that eq. (3.38) is actually in agreement with eq. (3.35).

The examples considered above reveal what makes it possible to construct an effective potential for systems describing the interaction between two degrees of freedom (e.g., spin and Bose operators, two spins, etc.). The structure of the Hamiltonian should allow the existence of an integral of the motion, with respect to the values of which the whole space of states may be classified. In each multiplet the matrix Schrödinger equation becomes one dimensional though the initial system is a two-particle system. This allows one, by introducing the corresponding generating function, to obtain a Schrödinger equation with a certain effective potential, provided that the matrix equation can be reduced to a form in which the coefficients are polynomials in a discrete variable of order not higher than two.

Next we present a few more examples without a detailed discussion. Let us consider two interacting oscillators

$$
H = \omega a^+ a + \Omega b^+ b + g(a^+ b^2 + a b^{+2})\,. \tag{3.40}
$$

Here the integral of the motion is

$$
R = 2a^+ a + b^+ b\,, \tag{3.41}
$$

the potential being

$$
\begin{aligned}
&U = \tfrac{1}{16}x^6 - \tfrac{1}{8}\nu x^4 + x^2(\tfrac{1}{16}\nu^2 - \tfrac{1}{2}R - \tfrac{3}{4}) + \tfrac{1}{2}\nu(R + \tfrac{1}{2})\,,\\
&\nu = (\omega - 2\Omega)/g\,, \qquad \kappa = (\Omega R - E)/g\,.
\end{aligned}
\tag{3.42}
$$

Consider now a system with a spin–spin (spin–orbit) interaction,

$$H = \alpha S_z^2 + \beta L_z^2 + \gamma L_z S_z + A S_z + B L_z + g(L_x S_x + L_y S_y) . \tag{3.43}$$

Here S_i and L_j correspond to angular momenta with magnitude S and L.

In general, a potential for the Hamiltonian (3.43) can be expressed in terms of elliptical functions, but this is quite cumbersome. We therefore restrict ourselves to some particular cases.

Let first $g = \alpha + \beta - \gamma$. Then the potential (up to a constant) is

$$\begin{aligned} U &= A_1 \sin^{-2} r + A_2 \cos^{-2} r + A_3 \sin^2 r + A_4 \sin^4 r , \\ A_1 &= (L - S - R)^2 - \tfrac{1}{4} , \qquad A_2 = (S - R - L)^2 - \tfrac{1}{4} , \\ A_3 &= -\frac{4(2S + 2L + 1)[A - B + R(\alpha - \beta)]}{g} , \\ A_4 &= -\frac{4[A - B + R(\alpha - \beta)]^2}{g^2} . \end{aligned} \tag{3.44}$$

The eigenvalue κ entering eq. (3.35) is $\kappa = -8E/g$.

Of special interest is the isotropic Heisenberg model,

$$H = \boldsymbol{S} \cdot \boldsymbol{L} . \tag{3.45}$$

As the calculations performed according to the above described plan show, this model is characterized by the generalized Eckart potential

$$U = [(R + S - L)^2 - \tfrac{1}{4}] \sinh^{-2} r + [\tfrac{1}{4} - (L + R - S)^2] \cosh^{-2} r . \tag{3.46}$$

Although the corresponding potential model is exactly solvable, it can be regarded as a limiting case of quasi-exactly solvable models [Turbiner 1988a].

Curiously, the well-known potential (3.46) gets, owing to the relation with the Heisenberg model, a group theoretical interpretation from yet another viewpoint (compare Alhassid et al. [1983]).

Note that the description of the spin system (3.45) with the aid of a potential is rigorous, in contrast to the known relation (in another sense) between the Heisenberg Hamiltonian and the Hamiltonian of a hydrogen molecule [Heitler and London 1927].

The potentials (3.44) and (3.38) turn out to be generalizations of potentials listed by Turbiner [1988a, b] due to the terms $\sinh^{-2} r$, $\sin^{-2} r$.

The generating function for the system (3.43) has the form

$$\Phi = \sum_{n=n_1}^{n_2} b_n z^n , \quad n_1 = \min(0, S + R - L) , \quad n_2 = \min(2S, S + L + R) . \tag{3.47}$$

Thus the potential models for which exact solutions can be found only for a finite number of states were successfully analysed from a common viewpoint. This concerns both the algebraic structure and the physical implications: They all obtain an immediate interpretation related to the very peculiarity of

their "emerging", being itself a rather unusual tangle of group theoretical and application matters. Moreover, the non-Hermiticity of the spin Hamiltonian corresponding to equations of the type (3.30) [Turbiner 1988c; Zaslavskii 1990a] is not an obstacle for such a physical interpretation since these operators and the corresponding matrix equations arise as auxiliary structures at intermediate stages. The resulting Schrödinger equation is Hermitian in coordinate space.

The potentials discussed in this section can be applied in the quantum theory of magnetism, the theory of interacting two-level systems with radiation, atomic and molecular physics, etc.

To conclude this section, we make some historical comments on the discovery of the potentials under consideration and their relation to spin systems.

Quantum mechanical potential models for which exact solutions exist for only a part of the energy spectrum were first obtained by Razavy [1980, 1981] (an example of the relation between a pseudospin model, viz. the Dicke model, and a second-order differential equation was found even earlier by Scharf [1974, 1975]). In papers we participated in [Zaslavskii et al. 1983; Zaslavskii and Ulyanov 1984] they were refound and generalized to the case of asymmetric potentials; there the correspondence with a spin system was established*).

The more general case leading to periodic potentials which can be expressed in terms of elliptic functions has been considered in our paper [Zaslavskii and Ulyanov 1987]; it corresponds to a general form of the quadratic–linear Hermitian spin Hamiltonian**).

In Turbiner [1988a, b] systems of the considered type (there called quasi-exact) were found again, including a series of new systems, e.g., the potential of a sextic anharmonic oscillator [Turbiner and Ushveridze 1987]. Besides, in Turbiner [1988c] the relation to the SL(2) algebra was rediscovered and the general case of a non-Hermitian quadratic–linear spin Hamiltonian was considered. An analogous issue was discussed by Zaslavskii [1990a], where such solutions were analysed mainly on the basis of difference equations.

4. Quantum tunnelling in spin systems and the effective potential method

4.1. Tunnelling splitting of energy levels

As has been shown in section 2, the correspondence between an anisotropic spin system and a particle moving in a potential field turns out to be an obvious and fruitful tool for investigating the magnetic properties of the spin system, specifically, the magnetization, susceptibility, etc. In this section, using the effective potential method, we analyse the problem of quantum tunnelling in spin systems, which is of interest by itself.

Let us consider such a system with a doubly degenerate classically ground state. Allowance for quantum effects may lead to removal of degeneracy and to energy level splitting, as in the case of a potential with two minima. Moreover, the frequency of transitions between classically degenerate states is determined by the magnitude of the splitting.

The investigation of tunnelling effects in different fields of solid state physics, which has been carried

*) They were refound once more by Scharf et al. [1987] in a study of spin tunnelling in spin systems (see next chapter). In the paper by Bagrov et al. [1988] it was stated that a new potential of the considered type was discovered; however, this case can actually be reduced to the ones already considered in our paper [Zaslavskii and Ulyanov 1984] by a simple change of variable (in this connection, see Zaslavskii [1990a]).

**) In a particular case the Lamé equation can thus be obtained; using the SL(2) algebra its group theoretical aspects were also analysed by Patera and Winternitz [1973], Miller [1977], Alhassid et al. [1983], Turbiner [1989] and Ward [1987].

out so intensively during recent years [Leggett et al. 1987], is mainly related to the study of particle interaction in a two-well potential with its surroundings serving as a heat bath (tunnelling splitting of the ground state being described with spin 1/2). Here we also deal with another kind of tunnelling caused by the quantum nature of the spin itself, whose value is supposed to be large enough.

These phenomena aroused interest quite recently because of both the need to develop special methods for the description of the quantum properties of spin systems [Van Hemmen and Süto 1986a, b; Enz and Schilling 1986a, b; Scharf et al. 1987; Zaslavskii 1989, 1990b, c] and the general physical issue of macroscopic tunnelling in magnetic systems, for instance, in small ferromagnetic particles [Chudnovsky and Gunther 1988a, b; Caldeira and Furuya 1988].

In order to calculate spin tunnelling, van Hemmen and Süto [1988a, b] and Scharf et al. [1987] used a WKB approximation yielding a relatively low accuracy for low-lying states. Enz and Schilling [1986a, b] employed a representation for spin operators in terms of a phase operator; this causes certain complications [Carruthers and Nieto 1968] and makes an estimate of the accuracy more difficult. In the paper by Chudnovsky and Gunther [1988a] an instanton technique was used which allows for contributions of subbarrier trajectories to the transition amplitude; however, only an exponential factor was calculated. Since in deep tunnelling the spin S enters the exponent, the difference between S and, for instance, $S + \frac{1}{2}$ can turn out to be essential in calculating the preexpontial factor.

We develop here a simple and obvious method of calculating the tunnelling splitting [Zaslavskii 1990b]. It is based on the above discussed correspondence between spin and conventional quantum mechanical systems. On the one hand, it clarifies the tunnelling picture and, on the other hand, allows the direct use of well-developed methods of quantum mechanics. This method enables one to compute the splitting not only of the ground state but also of excited states, and to describe the level splitting in the range of magnetic fields for which tunnelling is not exponentially small.

Let us first consider a spin system with anisotropy of the "easy-axis" type placed in a transverse magnetic field described by Hamiltonian (2.1). The energy spectrum of such a system coincides with the $2S + 1$ lowest-lying levels of a particle moving in the potential (1.9). If $B < B_0 = (2S + 1)\alpha$, the potential has two minima $x_\pm$ corresponding to the degenerate classical ground state (fig. 1a). This spin–coordinate correspondence allows one to compute the tunneling splitting taking advantage of the instanton technique [Coleman 1979; Weiss and Haeffner 1983]. In contrast to the paper by Enz and Schilling [1986a, b], in which instanton calculus was used in a rather complicated manner by reducing approximately the spin system to a Hamiltonian system on the basis of the phase operator introduced, the spin–coordinate correspondence allows one to introduce an obvious and rigorous definition of an instanton in the spin system.

The exponential factor is determined by the Euclidian action on a trajectory connecting both minima,

$$W = \int_{x_-}^{x_+} \mathrm{d}x \sqrt{2m(U - U_-)}\,, \tag{4.1}$$

where m is the particle mass, $U_- = U_+ = U(x_\pm)$, so that, in order to find the splitting with exponential accuracy, as was done in Chudnovsky and Gunther [1988a], one need not find the instanton trajectory in explicit form at all. However, it is necessary to determine the preexponential factor [Coleman 1979; Weiss and Haeffner 1983]

$$\Delta E_0 = \sqrt{\omega/\pi}\, A \exp(-W)\,. \tag{4.2}$$

Here ω is the frequency related to the potential minimum, $\hbar = 1$, and the constant A is defined from the relations

$$\begin{aligned} &\tau = \int_{x_m}^{x} \mathrm{d}x \sqrt{\frac{m}{2(U-U_+)}}\,, \\ &x(\tau) \simeq x_+ - \frac{A}{2\omega\sqrt{m}} \exp(-\omega\tau)\,, \quad \tau \to \infty\,, \end{aligned} \tag{4.3}$$

$x_m = 0$ corresponds to the midpoint of the potential between the two minima, τ is the Euclidian time. The instanton trajectory for the case at hand, eq. (2.1), can be found rather easily in explicit form,

$$\tanh \tfrac{1}{2}x = \sqrt{\frac{1-a}{1+a}} \tanh \tfrac{1}{2}\omega\tau\,, \quad \omega = \sqrt{1-a^2}\cdot B_0\,, \quad a = \frac{B}{B_0}\,, \tag{4.4}$$

from which, using formulae (4.1)–(4.3), we find

$$\Delta E_0 = \frac{8\alpha}{\sqrt{\pi}} \frac{(S+\frac{1}{2})^{3/2}(1-a^2)^{5/4}a^{2S}}{(1+\sqrt{1-a^2})^{2S+1}} \exp[(2S+1)\sqrt{1-a^2}]\,. \tag{4.5}$$

The introduced effective potential allows us, on the basis of the results of Weiss and Haeffner [1983], to obtain an expression for the splitting of the nth level,

$$\Delta E_n = \frac{q^n}{n!}\Delta E_0\,, \quad q = \frac{A^2}{2\omega}\,. \tag{4.6}$$

When one uses formula (4.6) for excited states, it should, however, be noted that this simple formula holds only for quadratic behaviour of the effective potential near the minimum up to the energy with the given n. These conditions are valid only asymptotically as $S \to \infty$. They do not hold for characteristic values of spins $S \sim 10$ for the effective potential (2.9) [of uniaxial spin systems (2.1)].

Notice that the effective potential method allows one to describe rather well the fine effect of spin energy level splitting on the basis of conventional approaches.

So, in order to compute the energy gap in the regime of deep (quasiclassical) tunnelling, i.e., when the transparency of the barrier separating the wells of the effective potential is exponentially small, one can take advantage of the standard Landau formula [Landau and Lifshitz 1977]

$$\Delta E_n = \frac{\hbar\omega}{\pi} \exp\left(-\frac{2}{\hbar}\int_0^{x_+} \mathrm{d}x\,|p|\right), \quad |p| = \sqrt{2m(U-E)}\,, \tag{4.7}$$

where the classical frequency ω of oscillations in a single well and the turning point correspond to the split energy level. This formula covers a sufficiently wide energy range providing very high accuracy. For the case of typical spin values $S \lesssim 20$ and magnetic fields up to the critical field B_0, the relative uncertainty is less than or equal to 1% for excited gaps and $\lesssim 5\%$ for the ground gap.

It should be noted that in Scharf et al. [1987] explicit formulae were obtained for the energy levels and energy gaps of uniaxial spin systems by explicit calculation of the subbarrier integral in a formula of the type (4.7) for $B \to 0$. Although these formulae yield good accuracy at small values of the magnetic field $B \leqslant 1$ (in the system of units with $\alpha = 1$), they are invalid for fields $B > 1$. Comparing the explicit formulae for the gap obtained in the framework of the effective potential method with instantons, eq. (4.6), and by the modified WKB method [Scharf et al. 1987], one comes to the following conclusions. Formula (4.6) covers almost the whole range of magnetic fields resulting in a stable relative uncertainty for the gap. So, for $S \sim 10$ the relative uncertainty turns out to be of the order of 10%, whereas the formulae of Scharf et al., eqs. (3.29) and (3.30), yield small uncertainties of the order of 1% only for extremely weak fields $B < 1$. In the range $B > 1$ these formulae fail (owing to the rapidly increasing uncertainties).

Comparison of the two approaches leads to the following conclusion. The advantages of the method used by Scharf et al. [1987] are the small uncertainties for weak fields and the explicit formulae obtained for the energies and gaps. The disadvantages are the rather cumbersome calculations to derive the formulae valid only for weak fields. As for the results (4.5), they are obtained in a very simple way, giving a stable accuracy for all values of the magnetic field in the regime of deep tunnelling. On the other hand, their disadvantage is that their validity is mainly restricted to the ground state, since the asymptotic formula (4.6) is practically invalid for excited gaps with spin values $S \sim 10$.

It should be noted that the Landau formula (4.7) does not hold in the range of energies close to the maximum of the barrier separating the wells (in the so-called critical energy range covering the range of fine tunnelling and overbarrier reflection). It is consistent to use here a combination of exact solution of the Schrödinger equation in the vicinity of the maximum of the potential with a conventional quasiclassical approximation away from the maximum. Such an approach, developed by one of the present authors [Ulyanov 1973, 1974], leads to modified energy quantization rules

$$\frac{1}{\hbar}\int_a^b \mathrm{d}x\, p = \pi n + \tfrac{1}{4}\pi + \alpha\,, \tag{4.8}$$

where the phase $\frac{1}{4}\pi$ is the contribution from the conventional turning point b, and the boundary phase α is the contribution from the barrier turning point a (in the case $E > U_{\max}$ the lower integration limit is chosen to be equal to zero, i.e., x_{m}).

The energy gap ΔE is determined by the solution of eqs. (4.8) for even, E^{g}, and odd, E^{u}, energy levels. It is essential that the corresponding boundary phases α^{g} and α^{u} are energy dependent. In particular, for the effective potential of interest, which can be fitted near the maximum by a parabola $U(x) \simeq U_{\mathrm{m}} - \beta x^2$ (a quadratic singularity), the following expressions are derived for the boundary phases [Ulyanov 1973, 1974, 1980]:

$$\alpha^{\mathrm{g}} = \tfrac{1}{8}\pi - \tfrac{1}{4}\lambda \ln(|\lambda|/4e) + \arg \Gamma(\tfrac{1}{4} + \tfrac{1}{4}\mathrm{i}\lambda)\,,$$

$$\alpha^{\mathrm{u}} = \tfrac{3}{8}\pi - \tfrac{1}{4}\lambda \ln(|\lambda|/4e) + \arg \Gamma(\tfrac{3}{4} + \tfrac{1}{4}\mathrm{i}\lambda)\,,$$

where Γ is the gamma function and $\lambda = (E - U_{\mathrm{m}})/\sqrt{\beta}$ is a dimensionless energy counted from the critical value (maximum of the potential). For boundary phases at $|\lambda| \ll 1$ we have series expansions with a logarithmic singularity,

$$\alpha^{g} = \tfrac{1}{8}\pi - \tfrac{1}{4}\lambda \ln|\lambda| + \tfrac{1}{4}\lambda(1 - \tfrac{1}{2}\pi - C - \ln 2) + O(\lambda^3),$$
$$\alpha^{u} = \tfrac{3}{8}\pi - \tfrac{1}{4}\lambda \ln|\lambda| + \tfrac{1}{4}\lambda(1 + \tfrac{1}{2}\pi - C - \ln 2) + O(\lambda^3), \tag{4.9}$$

C being the Euler constant.

Using the quantization formulae (4.8), in the critical energy range $|\lambda| \lesssim 1$ the energy gap can be computed with sufficiently high accuracy, specifically, the relative uncertainty does not exceed 2% for excited gaps and 6% for the ground gap for typical spin values $S \lesssim 20$.

As the magnetic field approaches the critical value $B_0 = 2S + 1$ the barrier between the effective potential wells becomes more transparent, vanishing at B_0. Owing to this effect, the tunnelling splitting of energy levels also disappears; at B_0 they form a spectrum typical for a potential with a fourfold minimum.

In the regime of deep tunnelling the quantization rules (4.8) give rise to the Landau formulae (4.7).

The energy spectrum of the spin problem under consideration has curious properties related to the existence of a critical range of energies. The effective potential method allows the most natural and obvious description of these properties on the basis of the general theory of quasiclassical approximations for special cases [Ulyanov 1973, 1974].

The quasiclassical approximation works here in an unusual way; namely, as the energy increases, the standard quasiclassical formula $\Delta E_n = \hbar\omega_{cl}$ proves to be insufficient to describe the structure of the energy spectrum (the classical frequency becomes zero at the critical energy). In this case one should take into account the detailed singular behaviour of the potential near a maximum. In the mass of energy levels an islet is formed which is a critical range where the modified quasiclassical energy quantization rules make allowance for an unusual energy dependence of the boundary phases. In the case of a symmetrical double well potential the problem is reduced by splitting into even and odd energy levels, for which one gets two different conditions in the center of the potential: First, the derivative of the wave function in the maximum of the potential becomes zero (the boundary condition for a "half-potential") for the even energy levels; secondly, the wave function itself becomes zero (impenetrability boundary condition) for the even levels.

A typical situation is presented in fig. 9, which corresponds to a spin S=10 and a magnetic field $B \simeq 12$ far away from the critical value $B_0 = 21$. The ground and first excited energy levels lie in the deep tunnelling regime, resulting in an exponentially narrow ground gap, whereas the second and third excited levels lie in the vicinity of the critical energy value (maximum of the potential); this results in a

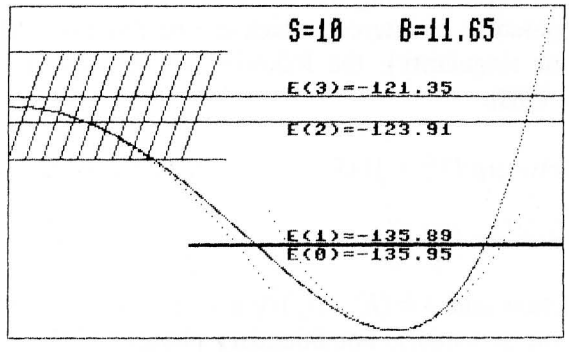


Fig. 9. Spin tunnelling in the critical energy range.

sufficiently wide gap (the critical range of energies is dashed). The remaining 17 energy levels are higher, corresponding to an equidistant energy spectrum.

In the intermediate energy range (a critical range in which the transition from deep to fine tunnelling and overbarrier reflection actually occurs) is nonquasiclassical with the gap width becoming comparable with the distance between gaps. It should be added that for typical spin values $S = 10$ only a few energy levels appear to lie in this critical range.

As a specific example, let us consider the case when the critical energy $U(0)$ lies precisely between the energy levels forming the gap at hand. Then, using formula (4.8) with the expansions (4.9) taken into account, we get the following explicit expression for the gap:

$$\Delta E = \pi\beta^{1/2}/(\ln \beta^{1/2} + \delta)\,. \tag{4.10}$$

Here $\beta = \frac{1}{4}B(B_0 - B)$ determines the quadratic behaviour of the effective potential near its maximum, $U(x) \simeq U(0) - \beta x^2$, and $\delta = C + 7\ln 2 + \ln(1 - B/B_0)$, C being the Euler constant.

As a comparison with numerical calculations of the gaps demonstrates, for $B \simeq B_0/2$ the calculation by this formula results in a relative uncertainty which does not exceed 5% in magnitude for spin values S varying from 1 to 100.

As for very large values of the spin, $S \gg 100$, when the quantity δ in the denominator of eq. (4.10) can be neglected, we come to the expression

$$\Delta E = \pi\beta^{1/2}/\ln \beta^{1/2}\,.$$

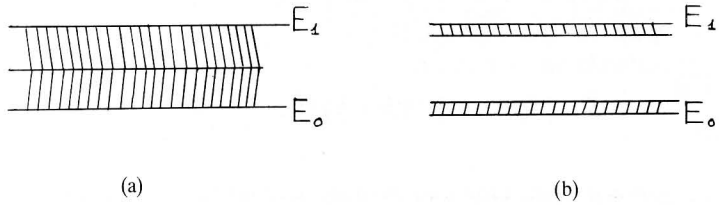
In particular, for $B = B_0/2$ the result is very simple,

$$\Delta E = \frac{\pi}{2}\,\frac{S}{\ln S}\,. \tag{4.11}$$

Next, let us consider the case of biaxial anisotropy with a Hamiltonian of the form (3.1). In this case the effective potential, as discussed in section 3, is periodic and the energy spectrum is related to the band structure.

Analyse first the case $B = 0$ assuming S to be integer (for half-integer S the degeneracy does not disappear, see section 2.3). Then the spin energy levels correspond to the edges of the merged bands (see fig. 10a). Therefore the splitting of the ground level of the spin system, $\Delta E_0 = E_1 - E_0$, equals the ground band width in the potential

$$U(x) = -\frac{\alpha\beta S(S+1)\,\mathrm{sn}^2 x}{\alpha + \beta\,\mathrm{cn}^2 x}\,, \tag{4.12}$$



(a) (b)

Fig. 10. Spin levels in the energy band picture for (a) $B = 0$ and (b) $B \neq 0$.

which follows from eq. (3.12) for $B = 0$. The quasiclassical band width can be computed by the instanton method [Coleman 1979], as was done in the case of tunnelling level splitting in a well [as compared to formula (4.2), an additional factor 2 arises]. An instanton trajectory (for instance, in a cell with $-K \le x \le K$) has the form

$$\operatorname{sn} x = \tanh(2\sqrt{\beta/(\alpha+\beta)}\,\tau)\,, \tag{4.13}$$

and the splitting proves to be equal to

$$\Delta E_0 = \frac{16}{\sqrt{\pi}}\,\tilde{S}^{3/2}\,\frac{(\alpha+\beta)^{3/4}\beta^{3/4}}{\alpha^{1/2}}\left(\frac{\sqrt{\alpha+\beta}-\sqrt{\beta}}{\sqrt{\alpha+\beta}+\sqrt{\beta}}\right)^{\tilde{S}}, \quad \tilde{S} = \sqrt{S(S+1)}\,. \tag{4.14}$$

For $\beta \ll \alpha$ the barrier between two neighbouring wells becomes transparent, the instanton method fails, and the behaviour of the system turns out to be essentially quantum mechanical. In this case the dynamics of the spin system whose initial state refers to the ground state can be found using the results of Glazman [1979] and Zaslavskii [1983],

$$\langle S_x(t)\rangle = S(\cos \alpha t)^{2S-1}\,. \tag{4.15}$$

The time dependence of the magnetic moment is essentially anharmonic; for $S \gg 1$ it is characterized by sharp bumps near the classical equilibrium positions.

Let us consider the other particular case, $B = 2\sqrt{\alpha\beta S(S+1)}$, such that the first term in the potential (3.12) becomes zero (the necessary condition for the double minimum to exist being $\beta > \alpha$). The spin ground state lies in the first energy band, whereas the first excited state lies in the second one (fig. 10b), as has been explained in section 3.1. If the barrier is sufficiently wide (it is always so for large S except when α and β are very close to each other), then the widths of the low-lying bands are negligible compared to the distance between them. This suggests that one need not be concerned with the detailed arrangement of the levels inside the band, i.e., one may neglect the behaviour of the spectral band related to the spacing of the potential. Then the difference between the energies of the first excited and ground spin levels can be computed immediately as the level splitting in a single cell from formulae (4.1)–(4.3). In so doing, it is sufficient to allow for the contributions of the instanton trajectory between the minima in the interior of the cell, as was done in the case of a conventional double well potential.

Let us list the expressions for the instanton trajectory and the value of the splitting,

$$\frac{1+\operatorname{cn} x}{1-\operatorname{cn} x} = \left(\frac{\sqrt{\beta}-\sqrt{\alpha}}{\sqrt{\beta}+\sqrt{\alpha}}\right)\tanh^2\left(\sqrt{\frac{\beta-\alpha}{\beta+\alpha}}\,\tau\right),$$

$$\Delta E_0 = \frac{4\sqrt{2}}{\sqrt{\pi}}\,\tilde{S}^{3/2}\,\frac{(\alpha+\beta)^2}{\sqrt{\alpha\beta}}\left(\frac{\sqrt{\alpha+\beta}-\sqrt{\beta-\alpha}}{\sqrt{\alpha+\beta}+\sqrt{\beta-\alpha}}\right)^{\tilde{S}} e^{2\varphi\tilde{S}}, \tag{4.16}$$

$$\varphi = \arccos\sqrt{\frac{\alpha+\beta}{2\beta}}\,, \qquad \tilde{S} = [S(S+1)]^{1/4}(S+\tfrac{1}{2})^{1/2}\,.$$

Finally, consider the general case. One can manage to find the instanton trajectory and to calculate the Euclidean action only if the potential (4.12) neglects the difference between $S(S+1)$ and $(S+\frac{1}{2})^2$,

which does not essentially affect the exponential dependence. The double minimum exists, provided that $B < \beta(2S+1)$. Let us present here the result of the calculations (with allowance made for the instanton contributions both between two minima in one cell and between two separate cells),

$$\Delta E_0 = \frac{16\beta}{\sqrt{\pi}} (S+\tfrac{1}{2})^{3/2}(b+a^2)^{-1/2}(1-a^2)^{5/4}(1+b)^{3/4}\left(\frac{\sqrt{1+b}-\sqrt{1-a^2}}{\sqrt{1+b}+\sqrt{1-a^2}}\right)^{S+1/2} \cosh\left(\pi \frac{a}{\sqrt{b}} \tilde{S}\varphi\right)$$
$$\times \exp\left[-2\tilde{S}ab^{-1/2} \tan^{-1}\left(\frac{a\sqrt{1+b}}{\sqrt{b(1-a^2)}}\right)\right], \tag{4.17}$$
$$\varphi = \arccos \frac{a\sqrt{1+b}}{\sqrt{a^2+b}}, \qquad \tilde{S} = S + \tfrac{1}{2}.$$

Note that in the above formulae for the energy splitting, eqs. (4.5), (4.14), and (4.17), the renormalized quantity $\tilde{S}$ enters instead of S, and that $\tilde{S}$ is different in different cases.

As far as formula (4.17) is concerned, it almost agrees with the one derived in another way in Enz and Schilling [1986b], eq. (16) (the difference is precisely related to the renormalization of the spin). One can convince oneself by direct calculation that both formulae agree in the limit $S \to \infty$. (This is not obvious in advance since the spin dependence has the structure $[f(S)]^S$ owing to the fact that the spin enters the definition of the parameter a via the critical field.) Numerical estimates show that formula (4.17) gives a two times larger relative uncertainty for the ground gap and spin values $S \sim 10$ than the corresponding formula (16) of Enz and Schilling [1986b]. Thus the advantage of formula (4.17), being the relative simplicity of its derivation based on the exact method of the effective potential in the framework of the spin–coordinate correspondence (in Enz and Schilling [1986a, b] the effective potential was introduced approximately), is compensated by the somewhat poorer accuracy as compared to the results of Enz and Schilling [1986b].

It should also be noted that in the vicinity of the critical field B_0 one can take advantage of the series expansion of the potential (see section 2.6) and get an especially simple expression for the tunnelling splitting,

$$\Delta E_0 = \alpha(S+\tfrac{1}{2})^{2/3} f(\gamma),$$
$$f(\gamma) = \frac{2^{17/4}}{\sqrt{\pi}} |\gamma|^{5/2} \exp\left(-\frac{2^{5/3}}{3}|\gamma|^{3/2}\right), \quad 1 \ll |\gamma| \ll (S+\tfrac{1}{2})^{2/3}. \tag{4.18}$$

The advantage of the effective potential method is that reduction of a spin system to the problem of a particle moving in a potential allows one to apply any adequate methods to study the energy spectrum, both analytical and numerical ones, known in quantum mechanics. Besides, the effective potential introduced allows one to deal immediately with a one-dimensional system rather than a two dimensional one (which may emerge, for instance, in parametrizing the classical spin with two spherical angles).

4.2. Spin tunnelling in a many-particle system

So far we considered tunnelling in systems described by a one-particle spin Hamiltonian. It is of

interest to investigate the more realistic case when the interaction between spins is taken into account. Let us consider here the Heisenberg model, which is of considerable physical interest [Vekslerchik et al. 1989]. Let the Hamiltonian be of the form

$$H = \alpha \sum_n S_n^{z^2} - \beta \sum_n S_n^{y^2} + B \sum_n S_n^x - J \sum_{n,\delta} \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+\delta} \,. \tag{4.19}$$

Here $J > 0$ is the exchange constant (the case of a ferromagnet), $\alpha \geq 0$ and $\beta > 0$ are the constants of the single-ion anisotropy and $\boldsymbol{\delta}$ labels the nearest neighbours.

In general, an investigation of the energy spectrum of such a Hamiltonian (in particular, of tunnelling for a degenerate ground state) encounters significant difficulties. We shall restrict ourselves to the case of weak anisotropy α and β and low values of B, when the one-ion part of the Hamiltonian can be regarded as a perturbation compared to the exchange part.

The ground state of an isotropic ferromagnet is known [Mattis 1965] to correspond to the maximal value of the total angular momentum $L = NS$ (N being the number of nodes), it is $(2L+1)$-fold degenerate with respect to its projection (say, L_z). Therefore in the first-order approximation the correction to the energy levels can be found from a secular equation, and the zeroth-order wave functions are constructed as follows:

$$|\Psi\rangle = \sum_{\sigma=-L}^{L} c_\sigma |\sigma\rangle \,, \quad L_z|\sigma\rangle = \sigma|\sigma\rangle \,. \tag{4.20}$$

Here only diagonal matrix elements and nondiagonal ones for the transitions $\sigma \to \sigma \pm 2$ are nonzero. Taking into account that

$$|\sigma\rangle = \sqrt{\frac{(L+\sigma)!}{(2L)!(L-\sigma)!}}\,(L_-)^{L-\sigma}|L\rangle \,, \tag{4.21}$$

where $L_- = L_x - \mathrm{i}L_y$ is a lowering operator, and applying the commutation rules for the spin components, we get for the diagonal matrix elements

$$f_\sigma = \langle\sigma| \sum_n S_n^{z^2} |\sigma\rangle$$

the following recursion relation:

$$f_\sigma = 2S\sigma - NS^2 + \frac{NS-\sigma}{NS+\sigma+1}\,[NS(S+1) + \sigma + 1 - f_{\sigma+1}] \,. \tag{4.22}$$

Its solution has the form

$$f_\sigma = \frac{2S-1}{2NS-1}\,(\sigma^2 - N^2S^2) + NS^2 \,. \tag{4.23}$$

The nondiagonal matrix elements can be calculated analogously.

As a result, the desired corrections, which correspond to the initial multiplet splitting, can be found as the eigenvalues of the Hamiltonian

$$H = \tilde{\alpha} L_z^2 - \tilde{\beta} L_y^2 + BL_x + \frac{N(N-1)}{2NS-1} S^2(\alpha - \beta) , \tag{4.24}$$

which describes a paramagnet with a spin $L = NS$ and anisotropy constants

$$\tilde{\alpha} = \alpha \frac{2S-1}{2NS-1} , \qquad \tilde{\beta} = \beta \frac{2S-1}{2NS-1} . \tag{4.25}$$

Thus one can say that the exchange interaction forms the resulting spin and leads to a renormalization of the anisotropy constants; however, it does not manifest itself immediately in the dynamical properties of the system in the given approximation for low-lying levels. The fact that for weak anisotropy and weak field, the initial many-particle system can be reduced to the one-particle system investigated above allows one, with a proper reformulation and change of notation for the parameters, to obtain formulae for tunnelling splitting by direct substitution into the corresponding formulae of the preceding section. One can thus not only get the tunnelling splitting for a ferromagnet, but also the energy itself of the ground state by analogy with section 2.6 for a paramagnet.

It should be noted that for $N \gg 1$ the condition of validity of perturbation theory for the energy values themselves, which is that the perturbation matrix elements are small compared with the level difference (in this case, of the magnon energy), is violated. However, for the level splitting ΔE_0 the obtained results remain valid also for $N \to \infty$ (being exponentially small in the effective spin), as, for instance, in the computation of the gap in superconductivity theory.

Above, single-ion anisotropy was considered. Consider now the case of inter-ion anisotropy for which the perturbative Hamiltonian has the form (for simplicity, we shall deal with a chain)

$$V = J_1 \sum_{n=1}^{N-1} S_n^z S_{n+1}^z - J_2 \sum_{n=1}^{N-1} S_n^y S_{n+1}^y . \tag{4.26}$$

Then, proceeding in analogy with the above argument, we find on the basis of perturbation theory that the effective Hamiltonian has the same structure (4.24), the effective constants of anisotropy being expressed in terms of the constants of the anisotropic part of the exchange interaction in the following manner:

$$\tilde{\alpha} = \frac{2S}{2NS-1} J_1(1 - N^{-1}) , \qquad \tilde{\beta} = \frac{2S}{2NS-1} J_2(1 - N^{-1}) . \tag{4.27}$$

[If both types of anisotropy are present, one should take the sum of the corresponding expressions (4.27).] Note that, apart from the different nature of quantum renormalization related to the own spins of the particles, the anisotropy constant contains now an additional factor. The latter allows for edge effects for a finite open chain (it becomes unity if the chain is closed).

Let us emphasize that all these factors, specifically quantum renormalization of the effective total angular momentum and the anisotropy constant also affected by the topology of the system, are essential owing to the strong exponential dependence in ΔE_0. A change of the number N by a finite amount may result in the appearance of additional factors of the order of unity. Therefore an experiment to determine the tunnelling transition frequencies $\Delta E_0/\hbar$ (for instance, in a study of small ferromagnetic particles) might be rather sensitive to the size of the interaction region.

As for the value of the exchange constant, the first-order approximation results do not depend on it at all. This point is related to the fact that the isotropic exchange part of the Hamiltonian commutes

with the total spin, rather than to the weak anisotropy approximation. Therefore it does not contribute to the momentum equation of motion as a whole (neither does it in the classical limit) and to the action for the corresponding instanton describing homogeneous precession in imaginary time (compare Chudnovsky and Gunther [1988a]). On the other hand, precisely these instantons make the main contribution to the transition amplitude, the definition of which is related to the calculation of tunnelling splitting [Coleman 1979] and result in macroscopic tunnelling.

Note that the derivation of the spin Hamiltonian (4.24) explicitly demonstrates the fact that in small ferromagnetic particles with a sufficiently strong exchange interaction the total magnetic moment can be regarded as a single quantum variable neglecting the details of the dynamics of the separate particles. In particular, this approximation can be used to describe macroscopic tunnelling [Chudnovsky and Gunther 1988a].

The quasiclassical condition for the tunnelling splitting formulae to be valid may actually be satisfied already for systems of finite size and relatively small spins of the particles $S \gtrsim 1$. The reason is that the product NS enters the tunnelling exponent determining the value of the collective angular momentum.

In this paper we do not discuss macroscopic tunnelling in continuous ferromagnetic systems [Chudnovsky and Gunther 1988b; Caldeira and Furuya 1988] and antiferromagnets [Krive and Zaslavskii 1990; Barbara and Chudnovsky 1990].

So we see that the results for tunnelling obtained by the effective potential method for one-spin systems actually turns out to be useful also in the case of many particles. Note that, besides the Heisenberg model, one can also mention in this connection the LGM model discussed in section 2.7. In this case the fermion coupling constants play the role of anisotropy constants. We shall not present here the corresponding formulae since they can be obtained from the above written ones by simple substitutions [Zaslavskii 1990e]. We only note that interest in the LGM model has increased very recently since its simplest generalization (interaction between three-level systems, not between two-level ones) turns out to be very useful in investigating quantum chaos [Meredith et al. 1988]. Therefore one may hope that the effective potential introduced for the LGM model and applied in the investigation of tunnelling may become the first step in constructing multidimensional potentials corresponding to finite-dimensional quantum systems in which chaos is possible.

4.3. Perturbation theory for tunnelling in a weak magnetic field

So far our consideration was based on the effective potential method. It has allowed us to apply different versions of the quasiclassical approach and to cover a rather wide range of magnetic fields and spin values. It turns out that in the case $B \to 0$ and arbitrary S the result for the tunnelling splitting considerably simplifies as compared to the general formulae listed in section 4.1. It also allows a generalization to spin Hamiltonians of a more complicated structure. In this case the calculation is based on the properties of the spin Hamiltonian; it does not require the introduction of the picture of a particle moving in a potential. The corresponding calculations are of some interest by themselves since they are rather rare practical applications to the case of the degeneracy being removed beginning from a rather high ($2S$th) order in the magnetic field.

Thus consider a spin system with the Hamiltonian (2.1) once more. Let the magnetic field $B \to 0$. The energy of the ground state and the first excited state (into which the ground level, which is degenerate in the absence of the field, splits) can be found from the perturbative equation

$$E = \varepsilon_S + \frac{V_{S,S-1}^2}{E - \varepsilon_{S-1}} + \cdots, \tag{4.28}$$

where the perturbation operator $V = -BS_x$ and $\varepsilon_\sigma = -\sigma^2$ indicates the level in which, for $B = 0$, the S_z-projection is equal to σ.

The double degeneracy of the energy levels of the nonperturbed Hamiltonian and the structure of the perturbation operator result in a perturbation series in powers of B for E_0 and E_1 in which the corresponding coefficients coincide in all orders $n < 2S$. The difference manifests itself starting from $N = 2S$. Therefore the tunnelling splitting value $\Delta E_0 = E_1 - E_0$ appears to be of order B^{2S}.

In order to determine ΔE_0 correctly, one needs to take into account explicitly the role of small denominators in "dangerous" terms of the series (4.28) by actually performing a partial summation of the perturbation series. This can be sketched as follows. Consider the leading "dangerous" term in the perturbation series

$$f = \frac{(V_{S,S-1}V_{S-1,S-2}\cdots V_{-S+1,-S})^2}{(E-\varepsilon_{S-1})(E-\varepsilon_{S-2})\cdots(E-\varepsilon_{-S+1})(E-\varepsilon_{-S})} . \tag{4.29}$$

If we introduce a sequence of points on a number axis from S to $-S$ corresponding to different values of σ, then this term corresponds to a single sequential transition from S to $-S$ and back. Now take into account that some elements of the number axis can be passed backward and forward a few times (after a transition from S to $-S$ the system returns to the intermediate point σ, then to $-S$ again and so on, passing the intermediate σ values). This suggests that additional factors appear in the perturbation series. Thus in the sum over terms which contain f as a common factor one should include higher orders of the perturbation. It is easy to guess that this will lead to the following form of the last retained term in the perturbation series:

$$f \to \tilde{f} = f(1 + r + r^2 + \cdots) = \frac{f}{1-r} , \quad r = \frac{1}{E-\varepsilon_S}\chi , \quad \chi = \frac{V_{-S,-S+1}V_{-S+1,-S}}{E-\varepsilon_{-S+1}} + \cdots . \tag{4.30}$$

The factor χ has the same form as the initial perturbation series (4.28), which allows one to construct a simple equation with respect to E:

$$\left(E - \varepsilon_S - \frac{V^2_{S,S-1}}{E-\varepsilon_{S-1}} - \cdots\right)^2 = \left(\frac{V_{S,S-1}V_{S-1,S-2}\cdots V_{-S+1,-S}}{(E-\varepsilon_{S-1})(E-\varepsilon_{S-2})\cdots(E-\varepsilon_{-S+1})}\right)^2 \equiv g_S^2 , \tag{4.31}$$

where the difference of the signs corresponds to the level splitting (the remaining terms coincide, making no contribution to the splitting). Thus, taking advantage of the explicit form of the matrix elements $V_{\sigma\sigma'}$, we get

$$\Delta E_0 = 2g_S \simeq (\tfrac{1}{2}B)^{2S} 8S^2/(2S)! . \tag{4.32}$$

For small spins $S \leq 3/2$ this result coincides with the exact value of $E_1 - E_0$ in the limit $B \to 0$ which was calculated using characteristic equations.

The formula obtained can be compared, for instance, with the limiting expression obtainable for $B \to 0$ from the formulae of Enz and Schilling [1986a, b]. It is easy to notice that in the latter, instead of the exact factor $(2S)!$ in eq. (4.32), its asymptotic value following from the Stirling formula appears. [Besides, the formula obtained by the effective potential contains an extra factor $(1 + 1/2S)^2$.]

As was done above for $\Delta E_0(\sigma = \pm S)$, one can obtain for the splitting of the nth level

$$\Delta E_n = 2(\tfrac{1}{2}B)^{2S-2n} \frac{(2S-n)!}{n!(2S-2n-1)!^2} . \tag{4.33}$$

Note that for $n \ll S$ this leads to an asymptotic form for the gap in agreement with formula (4.6) in the preceding section with $q = 32S^3/B^2$. In the very derivation the limited validity of formula (4.6) is apparent (for fields being not too small and numbers of levels being not too large), which becomes an obstacle for its practical application for $S \sim 10$ (as was mentioned above in the potential description language).

As far as formula (3.29) of Scharf et al. [1987] is concerned, for $n \ll S$ it results in an additional factor as compared with eq. (4.33),

$$\lambda_n = \left(\frac{\mathrm{e}}{2n+1}\right)^{n+1/2} \frac{2^n n!}{\sqrt{\pi}} .$$

The difference is relatively large for the ground level ($\sim 7\%$), but $\lambda_3 \simeq 0.9882$ already for $n = 3$.

The obtained results can easily be generalized to spin Hamiltonians of the form

$$H = -F(S_z) - BS_x , \tag{4.34}$$

where $F(x)$ is an even function increasing with x.

It should be noted that spin tunnelling for systems described by such Hamiltonians was investigated recently by Van Hemmen and Wreszinski [1988], who obtained inequalities and estimates for the tunnelling rate. The approach developed in the present section based on perturbation theory allows one to find explicitly the tunnelling splitting

$$\Delta E_0 = 2(\tfrac{1}{2}B)^{2S}(2S)!/\mu \tag{4.35}$$

(where S is chosen integer for definiteness),

$$\mu = \prod_{k=1}^{2S-1} [F(S) - F(S-k)] = F(S)\left(\prod_{m=1}^{S-1} [F(S) - F(m)]\right)^2 .$$

In the case of large $S \gg 1$ one can get an asymptotic estimate for ΔE_0. So, for $F(x) = x^{2p}$,

$$\Delta E_0 = (\tfrac{1}{4}BS\,\mathrm{e}^{1-c_p})^{2S} \frac{4p}{\sqrt{\pi}} S^{(8p-5)/2} , \quad c_p = \int_0^1 \mathrm{d}x \ln(1 + x^2 + \cdots + x^{2(p-1)}) . \tag{4.36}$$

For $p = 1$ we return again to the limiting form of the tunnelling splitting following from the effective potential method or the method of Enz and Schilling [1986b].

4.4. Metastable state decay

As was shown in section 4.1, the effective potential method allows one to draw a simple and obvious picture of quantum mechanical tunnelling in a spin system and to calculate the tunnelling splitting. Here we shall consider another situation related to metastable state decay, the temperature being finite [Zaslavskii 1989, 1990c].

Consider a spin system of the "easy-axis" type in an oblique magnetic field with a Hamiltonian (2.17), which corresponds, as we have seen in section 2.4, to the asymmetric potential (2.16). If $C \to 0$ and $B < B_0 = 2S + 1$, then the tunnelling splitting of the energy levels can be found by the approach of Weiss and Haeffner [1983] (see also Levine [1980]); it is given by

$$\delta E_n = \sqrt{\Delta E_n^2 + C^2(B_0^2 - B^2)}\,, \tag{4.37}$$

where ΔE_n is the tunnelling splitting in the absence of a longitudinal field, given by formula (4.5).

For a sufficiently high value of the longitudinal magnetic field $C \lesssim B_0$, provided that

$$D \equiv (B^{2/3} + C^{2/3})^{3/2} < B_0\,, \tag{4.38}$$

giving rise to the existence of a metastable state (see section 2.4 and fig. 2a), we deal with the problem of its decay. In general, it occurs due to both quantum and thermal fluctuations.

Consider first the decay caused by quantum mechanical tunnelling through a barrier. Then the probability density Γ_0 for the ground state of the left well, according to Weiss and Haeffner [1983], is equal to

$$\Gamma_0 = \sqrt{\frac{\omega}{\pi}}\,\frac{A}{2}\exp(-W)\,. \tag{4.39}$$

Here W is the total Euclidean action on the instanton trajectory going from x_0 to the turning point x_1 and back, ω is the frequency of small oscillations in the minimum x_0, and $\hbar = 1$. The constant A is determined from the asymptotic form of the instanton trajectory starting at $\tau \to -\infty$ in x_0, reaching the turning point x_1 at $\tau = 0$, and returning back to x_0 at $\tau = \infty$,

$$x(\tau) \underset{\tau\to\infty}{\simeq} x_0 + \frac{A}{2\omega\sqrt{m}}\exp(-\omega\tau)\,. \tag{4.40}$$

We confine ourselves to the case when the point which describes the system on the plane of the parameters B and C lies close to the astroid (4.38),

$$D = B_0(1-\delta)\,, \quad \delta \ll 1\,. \tag{4.41}$$

This allows us to fit the potential by the series expansion

$$U = U(x_0) + a(x-x_0)^2 - b(x-x_0)^3 + \cdots\,. \tag{4.42}$$

Then, after simple manipulations, we get

$$\Gamma_0 = \frac{8a^{7/2}}{b\sqrt{\pi}}\exp(-\tfrac{8}{15}a^{5/2}/b^2)\,, \qquad A = 2^{7/2}a^{3/2}/b\,, \qquad \omega = 2\sqrt{a}\,. \tag{4.43}$$

This expression holds for the potential (4.42) despite the specific problem it arises in. For the case at hand

$$a = \frac{3^{1/3}}{2^{2/3}}\,BC^{1/3}B_0^{2/3}\delta^{1/2}\,, \qquad b = \tfrac{1}{12}(B_0C)^{1/3}B^{4/3}\,. \tag{4.44}$$

Note that, although $\delta \ll 1$, for eq. (4.43) to be valid the dimensionless action should be $W \gg 1$, which may be satisfied due to the condition $S \gg 1$.

The spin system reduced to a particle moving in a potential also allows us, using the methods already developed, to determine the temperature dependence of the transition probability. According to Weiss and Haeffner [1983], at temperatures $T \lesssim \omega$

$$\frac{\Gamma(T)}{\Gamma(0)} = (1 - e^{-\omega/T}) \exp\left(\frac{A^2}{2\omega} e^{-\omega/T}\right), \tag{4.45}$$

from which, using eq. (4.43), we get

$$\frac{\Gamma(T)}{\Gamma(0)} = (1 - e^{-2\sqrt{a}/T}) \exp\left(\frac{32}{b^2} a^{5/2} e^{-2\sqrt{a}/T}\right). \tag{4.46}$$

For higher temperatures one can take advantage of the results of Affleck [1981], who used a WKB approximation,

$$\Gamma = \frac{\sqrt{a}}{\pi} \frac{\sinh \beta\sqrt{a}}{\sin \beta\sqrt{a}} \exp(-\tfrac{4}{27} a^3/Tb^2), \quad \beta = T^{-1}, \quad T > T_0 = \sqrt{a}/\pi . \tag{4.47a}$$

For $T \gtrsim T_0$,

$$\Gamma = \frac{1}{\pi} \frac{\sinh \beta\sqrt{a}}{(\pi/\sqrt{a} - \beta)} \exp(-\tfrac{4}{27} a^3/Tb^2) . \tag{4.47b}$$

For high temperatures with respect to ω classical thermal fluctuations prevail, and

$$\Gamma = \frac{\sqrt{a}}{\pi} \exp(-\tfrac{4}{27} a^3/Tb^2) . \tag{4.48}$$

Analogously, an expression for Γ can be obtained in the narrow crossover region between the quantum mechanical and thermal transitions in the immediate vicinity of T_0 [Affleck 1981]. However, it results in rather cumbersome expressions which will not be presented here.

Note that, although the coordinate system described by the potential (2.16) has overspin states with numbers $n > 2S$, for $T \ll \omega S \sim Sa^{1/2} \sim S^2\delta^{1/4}$ (for B and $C \lesssim B_0$) the relative contribution of these states to the calculated quantities is exponentially small.

As was done for the spin system of "easy-axis" type, metastable state decay can be analysed in the case of an "easy plane". Consider, for instance, the spin Hamiltonian

$$H = S_z^2 - BS_x , \tag{4.49}$$

which the potential (2.20) corresponds to. The metastable state exists, provided that $B > B_0 = 2S + 1$. In the effective potential language the point $\varphi = 0$ corresponds to it (in a proper cell). For $B - B_0 \ll B_0$ the potential can be expanded in powers of the coordinate (as was done above). Now this expansion incorporates terms of the second and fourth orders,

$$U(\varphi) \simeq U(0) + a\varphi^2 - b\varphi^4 . \tag{4.50}$$

In expression (4.39) (e.g., for tunnelling through the barrier in one direction) we now have

$$W = \tfrac{2}{3}a^{3/2}/b\,, \qquad \omega = 2\sqrt{a}\,, \qquad A = 2^{5/2}a/\sqrt{b}\,. \tag{4.51}$$

For $T < T_1 = (1/2\pi)\sqrt{B^2 - B_0^2}$ the temperature dependence of $\Gamma(T)$ is determined by formula (4.45). For the system determined by the Hamiltonian (4.49) the coefficients a and b are

$$a = \tfrac{1}{4}B(B - B_0)\,, \qquad b = \tfrac{1}{48}B(4B - B_0) \simeq \tfrac{1}{16}B_0^2\,. \tag{4.52}$$

For $T \gtrsim T_1$

$$\Gamma = \frac{TT_1}{\pi(T - T_1)} \sinh(\omega/2T)\exp(-T_2/T)\,, \quad T_2 = \tfrac{1}{4}(B - B_0)^2\,, \tag{4.53}$$

and for $T \gg T_1$

$$\Gamma = \frac{\sqrt{B(B - B_0)}}{2\pi}\exp(-T_2/T)\,. \tag{4.54}$$

The more complicated case of biaxial anisotropy can be treated in an analogous way.

Strictly speaking, the obtained formulae describe the decay process in the time range $t \sim \Gamma^{-1}$. In general, a reflection from the effective potential walls occurs, and in thermodynamic equilibrium the probability of the transition from left to right is compensated by the flux from right to left, being equal in magnitude and opposite in direction. The above obtained formulae retain the same meaning for each flux separately if only the waves leaving through the barrier are taken into account [Noble 1979]. Note that, since metastable state decay can be described by introducing complex energies, the results listed in the present section actually generalize the spin–coordinate correspondence to the case of complex energies.

Thus we succeeded in describing tunnelling from a common point of view quite simply over a rather wide temperature range, with the limiting cases of purely quantum mechanical and thermal transitions incorporated.

Numerical estimates [Chudnovsky and Gunther 1988a] show that for values of the magnetization and the anisotropy constant per unit volume of $500\,\mathrm{emu/cm^3}$ and $5 \times 10^6\,\mathrm{erg/cm^3}$, respectively, the crossover temperature is $\lesssim 0.1\,\mathrm{K}$.

Of interest is an application of the developed formalism to the description of tunnelling in spin systems with allowance for dissipation, beyond the framework of the two-level approximation [Leggett et al. 1987; Ivlev 1988].

5. Quasiclassical approximation for spin systems

The goal of this section is to construct a quasiclassical approximation for spin systems of a sufficiently general form, to find quantum corrections to thermodynamical quantities, to derive Bohr–Sommerfeld energy quantization rules including corrections, and to study manifestations of quantum properties in the dynamics of spin systems [Zaslavskii 1984a, b, 1987].

When describing the properties of quantum spin systems one encounters difficulties caused by the difference between the commutation relations of momentum components and the corresponding coordinate–momentum relations. Therefore an immediate extension of the methods valid, e.g., for Bose systems, turns out to be unjustified for the general case of spin systems. As we have seen in the preceding sections, an effective potential can, however, be constructed for a wide variety of spin Hamiltonians, which allows one to take advantage of the well-developed formalism of "conventional" quantum mechanics.

Generally speaking, it is nonetheless insufficient to solve the stated problem of constructing a quasiclassical approximation. The considered type of spin Hamiltonian is not the most general. Besides, only one-spin Hamiltonians (or those reducible to them) were considered above. Meanwhile, most interest, e.g., to construct the Wigner–Kirkwood expansion, is aroused by the more realistic case of many-particle systems with an interaction between the spins.

Spin variables have a discrete nature. On the other hand, due to the very meaning of the quasiclassical approximation, the solution can be expressed in classical terms (for example, using angular variables). Therefore from the very beginning one must use a continuous representation of a quantum spin system. This can be done using spin coherent states introduced by Radcliffe [1971], which are a particular case of generalized coherent states [Perelomov 1972, 1986]. Above, in section 3, such states were used to construct the effective potential. At present we are speaking about yet another application of these states. Their use in problems related to the quasiclassical approximation seems natural because, in particular, these states are "most classical".

Note that the so-called semiclassical method, which allows one to introduce approximately for a spin system (with spin $S \gg 1$) coordinate and momentum-type variables, does not serve the stated purpose at all (or, at least, is not sufficient). Remember that the method considers small quantized oscillations of the magnetization against the background of the classical equilibrium state, i.e., the spin Hamiltonian is replaced by the Hamiltonian of a set of harmonic oscillators [Akhiezer et al. 1968]. Therefore, use of this method is difficult even in the simplest cases if the system is essentially nonlinear (see section 1.6). Besides, its validity is confined to low-lying states and low temperatures. One can say that in the semiclassical approach the zeroth-order approximation is a linear but quantum mechanical system, whereas in the quasiclassical approach it is a classical but nonlinear system.

5.1. Wigner–Kirkwood expansion for spin systems

Let us first consider a spin system in thermodynamical equilibrium, and derive for it an expansion of the statistical sum in inverse powers of the spin, S^{-1} (for $S \to \infty$ and $\hbar S = \text{const.}$ this is equivalent to an expansion in powers of $\hbar$). For simplicity, in the meantime let us regard the system as a one-particle system. When calculating the trace

$$Z = \operatorname{Tr} \exp(-\beta H) , \tag{5.1}$$

we take advantage of the completeness of spin coherent states $|\xi\rangle$. Then

$$Z = \int \mathrm{d}\mu \, \langle \xi | \exp(-\beta H) | \xi \rangle , \tag{5.2}$$

where the integration measure is

$$d\mu = \frac{2S+1}{\pi}\,\frac{d^2\xi}{(1+|\xi|^2)^2} = \frac{2S+1}{4\pi}\,d\varphi\,d\theta\sin\theta\,,$$
$$\xi = \tan\tfrac{1}{2}\theta\,e^{i\varphi}\,,\quad 0\le\theta\le\pi\,,\quad 0\le\varphi<2\pi\,. \tag{5.3}$$

Using the explicit form of normalized coherent states,

$$|\xi\rangle = (1+|\xi|^2)^{-S}\exp(\xi S_-)|S\rangle\,, \tag{5.4}$$

one can get for any arbitrary operator $\hat{f}$

$$\langle\xi|\hat{S}_i\hat{f}|\xi\rangle = \tilde{S}_i f\,,\quad f = \langle\xi|\hat{f}|\xi\rangle\,,$$
$$\tilde{S}_x = \frac{S(\xi+\xi^*)}{1+|\xi|^2} + \frac{1-\xi^{*2}}{2}\,\frac{\partial}{\partial\xi^*}\,,$$
$$\tilde{S}_y = \frac{S(\xi-\xi^*)}{i(1+|\xi|^2)} + \frac{1+\xi^{*2}}{2i}\,\frac{\partial}{\partial\xi^*}\,, \tag{5.5}$$
$$\tilde{S}_z = \frac{S(1-|\xi|^2)}{1+|\xi|^2} - \xi^*\,\frac{\partial}{\partial\xi^*}\,.$$

The first term in each $\tilde{S}_i$ coincides with Sn_i, where $\boldsymbol{n}$ is the unit vector defined by the angles θ and φ related to ξ and ξ^* according to eq. (5.3). The operator $\tilde{\boldsymbol{S}}$ possesses an especially compact form if written in terms of the components of $\boldsymbol{n}$,

$$\tilde{\boldsymbol{S}} = S\boldsymbol{n} + \tfrac{1}{2}(\hat{\boldsymbol{a}} - i\hat{\boldsymbol{b}})\,,$$
$$\hat{\boldsymbol{a}} = \boldsymbol{\nabla} - \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{\nabla}) \equiv -\boldsymbol{n}\times\hat{\boldsymbol{b}}\,,\qquad \hat{\boldsymbol{b}} = \boldsymbol{n}\times\boldsymbol{\nabla}\,,\quad \boldsymbol{\nabla}\equiv\partial/\partial\boldsymbol{n}\,. \tag{5.6}$$

It is easy to verify that the $\tilde{S}_i$ actually satisfy the commutation relations for a momentum and that $\tilde{\boldsymbol{S}}^2 = S(S+1)$. Note that expressions analogous to eq. (5.5) were used in terms of angular variables by Narducci et al. [1975], called D-operator calculus, in their investigation of superradiation of systems.

If we confine ourselves to the unit circle $\xi = e^{i\varphi}$, then we come again to the representation (3.6) used in section 3.1 to construct the effective potential.

Using eqs. (5.5) and (5.6), one can find that the quantity $Q = \langle\xi|\exp(-\beta H)|\xi\rangle$ satisfies the closed differential equation

$$\partial Q/\partial\beta = -H(\tilde{S})Q\,, \tag{5.7}$$

with the initial condition $Q|_{\beta=0} = 1$. In addition to eq. (5.7), the quantity Q also satisfies the complex conjugate equation. It is most convenient to treat their half-sum, which explicitly reflects the reality of Q. The equivalence of the solutions of these equations is immediately apparent due to the fact that the commutator $[\tilde{S}_i, \tilde{S}_j^*] = 0$ and

$$H(\tilde{S})\cdot 1 = \langle \xi | H | \xi \rangle = H^*(\tilde{S})\cdot 1 .$$

Then one gets for the statistical sum the expression

$$Z = \frac{2S+1}{4\pi} \int \mathrm{d}O \exp(-\beta \hat{L})\cdot 1 , \quad \mathrm{d}O = \mathrm{d}\varphi \, \mathrm{d}\theta \sin\theta , \quad \hat{L} = \mathrm{Re}\, H(\tilde{S}) . \tag{5.8}$$

It is exact and applicable to an arbitrary spin, and it allows a direct generalization to the case of many-particle systems.

Let $S \gg 1$. Then an expansion of eq. (5.8) in $\hat{\boldsymbol{a}}$ and $\hat{\boldsymbol{b}}$ results in an expansion of the statistical sum in powers of S^{-1}. The leading-order approximation is given by neglecting the operator part $\tilde{\boldsymbol{S}}$ and corresponds to the classical expression, for which one can neglect the noncommutativity of the different components of the spin. In other words, the Wigner–Kirkwood expansion is constructed as a perturbation series in derivatives with respect to the classical spin components.

Consider first the one-particle system described by the general Hamiltonian

$$H = f(\boldsymbol{S}) . \tag{5.9}$$

Then the leading-order quantum correction is

$$\delta F = \tfrac{1}{4} S^{-1} \sum_{k,l} \langle (\delta_{kl} - n_k n_l)(f_{,k,l} - \beta f_{,k} f_{,l}) \rangle . \tag{5.10}$$

Here δ_{kl} is the Kronecker delta, $f_{,k} = \partial f / \partial n_k$, angular brackets indicate averaging over the classical Gibbs distribution with the corresponding classical Hamilton function $f(S\boldsymbol{n})$. Let us pay attention to the fact that, in contrast to systems described by variables of the type of conventional coordinates and momenta [Landau and Lifshitz 1969], here the first nonzero correction arises already in the lowest-order approximation. It should be noted that the expression for the correction is unambiguously determined by the classical Hamilton function despite the order of the operators in the Hamiltonian (5.9). The corrections related to this order manifest themselves in higher orders in S^{-1}.

The next example refers to the isotropic Heisenberg chain, which is one of the simplest spin models describing the properties of magnetic dielectrics [Mattis 1965]. In the framework of this model a series of exact results were obtained for stationary states: the Bethe solution for $S = 1/2$ [Bethe 1931], the ground state, and one- and two-magnon states of ferromagnetic systems with arbitrary spins are known [Mattis 1965]. However, one cannot obtain a sufficiently simple expression for the statistical sum which is convenient to study thermodynamical properties. The model statistical sum can be calculated exactly only in the classical limit, in which the spin is replaced by a c-number vector of fixed length [Fisher 1964].

It should be noted that thermodynamical properties of the Heisenberg quantum model were investigated by Lieb [1973] who established thermodynamical inequalities for quantum spin systems, the spin values considered being arbitrary. Kolokolov [1986] obtained a functional integral representation for the Heisenberg statistical model in closed form. Tsuzuki [1985, 1986a] used a spin coherent state representation to develop the method of the transfer matrix in a form convenient for numerical calculations in application to the X–Y and isotropic Heisenberg chains. However, the methods developed in these papers do not give a constructive procedure for immediate calculation of quantum

corrections for $S \gg 1$. Tsuzuki [1984] applied an approach close to the one of Zaslavskii [1984b] to derive an effective Hamiltonian in the spin coherent state representation; however, a systematic expansion of thermodynamic quantities in powers of S^{-1} was not constructed.

The Hamiltonian of the isotropic Heisenberg chain reads

$$H = -J \sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i-1} . \tag{5.11}$$

Applying the above described technique, the expression for the statistical sum can be written as

$$Z = (2S+1)^{N+1} \tilde{Z} , \quad \tilde{Z} = \int \frac{\mathrm{d}O_0}{4\pi} \prod_{i=1}^{N} \frac{\mathrm{d}O_i}{4\pi} \exp(\beta J \tilde{\boldsymbol{S}}_i \cdot \tilde{\boldsymbol{S}}_{i-1}) \cdot 1 . \tag{5.12}$$

The zeroth-order term of the expansion refers [up to a term $-T \ln(2S+1)$] to the classical result of Fisher [1964], according to which the free energy per site is

$$F_{\mathrm{cl}} = -T \ln \frac{\sinh k}{k} , \quad k = \beta J S^2 . \tag{5.13}$$

The first quantum correction is expressed through two- and four-point correlations,

$$\delta_1 F = -\frac{Tk^2}{4SN} \sum_{\alpha,\beta,m} \langle (\delta_{\alpha\beta} - n_{\alpha m} n_{\beta m})(n^{\alpha}_{m+1} + n^{\alpha}_{m-1})(n^{\beta}_{m+1} + n^{\beta}_{m-1}) \rangle , \quad \alpha, \beta = x, y, z . \tag{5.14}$$

The general form of the correction $\delta_2 F \sim S^{-2}$ is very cumbersome, it contains correlation functions of higher orders up to the eighth one. Two-point correlations were found by Fisher [1964] with the aid of a moving coordinate system (so that in each site the spin direction served as the polar axis for the next one). However, this method cannot be directly generalized to calculations of more complex correlations. It is more convenient here to take advantage of the transfer matrix method performing an integration over the edge spin variables in the corresponding averages. Omitting technical details of the calculations, we present here the expressions for some typical averages:

$$\begin{aligned}
&\langle \boldsymbol{n}_m \cdot \boldsymbol{n}_{m+l} \rangle = u^{|l|} , \\
&\langle (\boldsymbol{n}_m \cdot \boldsymbol{n}_{m+1})^2 \rangle = 1 - 2u/k , \\
&\langle \boldsymbol{n} \cdot \boldsymbol{p} \rangle_{\boldsymbol{n}_1} = (\boldsymbol{n}_1 \cdot \boldsymbol{p}) u , \\
&\langle (\boldsymbol{n} \cdot \boldsymbol{p}_1)(\boldsymbol{n} \cdot \boldsymbol{p}_2) \rangle_{\boldsymbol{n}_1} = (u/k)(\boldsymbol{p}_1 \cdot \boldsymbol{p}_2) + (\boldsymbol{n}_1 \cdot \boldsymbol{p}_1)(\boldsymbol{n}_2 \cdot \boldsymbol{p}_2)(1 - 3u/k) , \\
&\langle \cdots \rangle_{\boldsymbol{n}_1} = \frac{\int \mathrm{d}O_{\boldsymbol{n}} \exp(k \boldsymbol{n} \cdot \boldsymbol{n}_1)(\cdots)}{\int \mathrm{d}O_{\boldsymbol{n}} \exp(k \boldsymbol{n} \cdot \boldsymbol{n}_1)} ,
\end{aligned} \tag{5.15}$$

$\boldsymbol{p}_{1,2}$ being arbitrary fixed vectors, $u(k) = \coth k - k^{-1}$ is a so-called Brillouin function.

As a result, the first two quantum corrections turn out to be equal to

$$\delta_1 F = -(T/S)ku(k)\,,$$
$$\delta_2 F = \tfrac{1}{12}(T/S^2)(7u^2k^2 + k^2u + 9ku - 5k^2)\,. \tag{5.16}$$

Next we pay attention to the following. The expression for $\delta_1 F$ is proportional to $\partial F_{cl}/\partial k$. Therefore F_{cl} and $\delta_1 F$ are conveniently treated by introducing a new variable $q = \beta JS(S+1)$ instead of k. Then, with the considered accuracy, such a renormalized expression for the free energy is simplified, so that the leading-order quantum correction turns out to be (as was pointed out by Fisher [1964]) of order S^{-2},

$$\frac{F}{JS(S+1)} = -\frac{1}{q}\ln\left(\frac{(2S+1)\sinh q}{q}\right) + \frac{1}{12S^2}\left[q(1+u+u^2) - 3u\right], \quad u = u(q)\,. \tag{5.17}$$

From the viewpoint of spin coherent states, this renormalization suggests that the "classical" term in eq. (5.6) be chosen in the form $S_{eff}\boldsymbol{n}$, where $S_{eff} = [S(S+1)]^{1/2}$, which implies that allowance is made for the quantization of the momentum squared already in the leading order.

The first term in eq. (5.17) [and in the purely classical expression (5.13) as well] is an even function of q; hence there is no difference between ferromagnetic and antiferromagnetic systems. It manifests itself in the quantum correction. Consider first the ferromagnetic case $J > 0$. Then the correction in eq. (5.17) is positive for any q (just like for conventional Hamiltonian systems [Landau and Lifshitz 1969]). Therefore, if one uses Lieb inequalities [Lieb 1973], then

$$F_{cl}(\kappa) < F_{cl}(q) < F < F_{cl}(k)\,, \quad \kappa = \beta J(S+1)^2\,. \tag{5.18}$$

For an antiferromagnetic system ($J < 0$)

$$\frac{\delta_2 F}{|J|} = \frac{|q|(1-u+u^2) - 3u}{12}\,, \quad u = u(|q|)\,. \tag{5.19}$$

In the high-temperature limit, where $q \to 0$, then

$$\delta_2 F/|J| \simeq -\tfrac{1}{36}q^2\,.$$

For $|q| \gg 1$ (but with the temperature not low enough to violate the validity of the quasiclassical approximation), then

$$\delta_2 F/|J| \simeq \tfrac{1}{12}|q|\,.$$

In the intermediate point $|q| \simeq 2.34$ the correction $\delta_2 F$ becomes zero. For $|q| > |q_1|$ an estimate analogous to eq. (5.18) holds. If $|q| \le |q_1|$, then

$$F_{cl}(\kappa) < F \le F_{cl}(q)\,. \tag{5.20}$$

Thus the quasiclassical expansion turns out to be especially efficient for an antiferromagnetic chain in the vicinity of $q = q_1$, where the quantum term of order S^{-2} becomes zero and quantum corrections are of higher order.

For the obtained formulae to be valid, the temperature should be high enough, viz., $T \gg JS$ (or, which is the same, $|q| \ll S$, although q itself need not be small). If $q \to 0$, then the corresponding expressions go to the results of the direct expansion of the exponential function in eq. (5.12) in powers of the inverse temperature. In the temperature range $JS \ll T \ll JS^2$ the expression for the energy related to eq. (5.17) coincides with the one given by the spin-wave approximation, i.e., a conventional quasiclassical approach holds [Akhiezer et al. 1968].

5.2. *Energy quantization rules for the spin Hamiltonian in a nonfunctional approach*

Let us consider now a derivation of the energy quantization rules. The standard quantum mechanical derivation [Landau and Lifshitz 1977] is based on the solution of a differential equation or the construction of a path integral representation [Dashen et al. 1974]. It was realized for the case of spin systems by Klauder [1979] using spin coherent states. Energy quantization rules of the Bohr–Sommerfeld type (i.e., without quantum corrections) were set up for spin systems using continuous integration by Schankar [1980]. We use a much simpler and more constructive procedure which allows us to derive an exact relationship for the energy levels which upon expansion in a power series results in the quantization rules with the desired accuracy.

To do this, we take advantage of the approach developed by Ulyanov [1982] for "conventional" quantum mechanical systems, called there the nonfunctional approach. Following Ulyanov, we write an exact relationship for the number of states,

$$\Gamma(E_n) = \sum_k \theta(E_n - E_k) = \mathrm{Tr}\,\theta(E_n - H) = n + \tfrac{1}{2} \tag{5.21}$$

(for simplicity, degeneracy is assumed to be absent), where $\theta(x)$ is the Heaviside step function. Using the integral representation,

$$\theta(x) = \frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty+0}^{\mathrm{i}\infty+0} \frac{\mathrm{d}\beta}{\beta} \mathrm{e}^{\beta x}, \tag{5.22}$$

and expression (5.8), we get

$$\frac{2S+1}{4\pi} \int \mathrm{d}O\, \theta(E_n - \hat{L}) \cdot 1 = n + \tfrac{1}{2} \tag{5.23}$$

(the θ-operator is determined by the integral representation cited above). If there are degenerate energy levels, the right-hand side of formula (5.21) should contain the expression $N + \frac{1}{2} g(E_n)$, $g(E_n)$ being the multiplicity of the corresponding level, and $N = \Sigma_k\, g(E_k)$, where the sum runs over all levels k with $E_k < E_n$.

Equation (5.23) is exact. In essence, it expresses a relation between mechanics and statistics, information about Z being used to obtain the energy quantization rules (not vice versa). Specifically, it is the substitution of the Wigner–Kirkwood expansion of eq. (5.23) into Z that leads to the desired rules. Let the Hamiltonian have the general form (5.9), and let $S \gg 1$. Then, using the quasiclassical approximation for the trace $\mathrm{Tr}\exp(-\beta H)$ of the type (5.10), and taking into account that in the inverse Laplace transformation each power of β leads to a derivative $\partial/\partial E$, we obtain the quantization rules in which the leading term and the quantum correction to it are retained,

$$\frac{2S+1}{4\pi}\int \mathrm{d}O\,\theta(E-f)+\frac{1}{8\pi}\sum_{k,l}\int \mathrm{d}O\,(\delta_{kl}-n_k n_l)[f_{,k}f_{,l}\delta'(E-f)-f_{,k,l}\delta(E-f)]=n+\tfrac{1}{2}\,. \quad (5.24)$$

Here f is a classical Hamilton function referring to eq. (5.9).

In the zeroth-order approximation, integrating eq. (5.21) by parts, we get

$$\oint \frac{\mathrm{d}\varphi}{2\pi}\,S_z(\varphi, E)=n-S[\theta(E-f_+)+\theta(E-f_-)]\,,\quad f_\pm=f|_{S_z=\pm S}\neq E\,. \quad (5.25)$$

Here $S_z(\varphi, E)$ is a solution of the equation $f(S_z, \varphi)=E$, the integration is performed over one whole period of φ (taking into account the multivaluedness of $S_z(\varphi, E)$ in general) in the range constrained by the condition $|S_z(\varphi, E)|\leq S$.

One can make sure that for a Zeeman-type Hamiltonian $\boldsymbol{B}\cdot\boldsymbol{S}$, $\boldsymbol{B}$ being proportional to the magnetic field, formula (5.24) yields an exact result already in the leading-order approximation, as in the case of the harmonic oscillator in conventional quantum mechanics.

As follows from eq. (5.24), the quantization rules in the leading-order approximation mean that the number of states in phase space is equal to a given number. Meanwhile, the role of phase space is played by a sphere, and the elementary cell has size $2\pi S^{-1}$. Note that the meaning of the notion that spin coherent states are quasiclassical is thus defined more exactly; other aspects of this meaning were discussed by Perelomov [1972, 1986]. Strictly speaking, eqs. (5.24) and (5.25) lose their validity in the case of a multiply connected phase space when the energy value is close to the value of the effective potential barrier, as in the case of a particle moving in a two-hump potential well [Ulyanov 1973].

The use of spin coherent states also allows one to obtain relatively simply a quasiclassical expansion for Green functions, i.e., for matrix elements of the resolvent operator determined according to

$$(\hat{H}-z)\hat{G}=1\,. \quad (5.26)$$

Actually, averaging this equation over $|\xi\rangle$, we have

$$(f-z)G=[1-(L-f)]G\,,\quad L=H(\tilde{S})\,,$$

where $G=\langle\xi|\hat{G}|\xi\rangle$. In the representation of spin coherent states diagonal elements completely determine the operator.

For $S\gg 1$ we shall look for a solution in the form of a series,

$$G=\sum_{k=0}^{\infty}(S^{-1})^k G_k\,.$$

For a Hamiltonian of the form of eq. (5.9), we obtain for the first two coefficients

$$G_0=(f-z)^{-1}\,,$$

$$G_1=\tfrac{1}{2}G_0^3\sum_{k,l}f_{,l}f_{,k}(\delta_{kl}-n_k n_l)-\tfrac{1}{4}G_0^2\sum_{k,l}(\delta_{kl}-n_k n_l)f_{,k,l}\,.$$

If one makes use of the relation

$$\nu(E) = \frac{1}{2\pi i} \mathrm{Tr}[\hat{G}(E + i0) - \hat{G}(E - i0)]$$

for the density of states $\nu(E) = d\Gamma/dE$, then these equations yield a quasiclassical approximation of $\nu(E)$ which agrees with eq. (5.24).

The nonfunctional approach also allows one to obtain immediately in integral form (without referring directly to a Schrödinger equation) quasiclassical equations for the characteristics of the motion [Zaslavskii 1984b], as was done in the book by Ulyanov [1982].

Let us emphasize the following point. For systems for which the coordinate and momentum are dynamical variables, one need not use coherent states to construct quasiclassical expansions and to derive energy quantization rules [Landau and Lifshitz 1969, 1977; Ulyanov 1982] (though their use is possible resulting in a simplification of the relevant calculations for several cases). Meanwhile, it is just the reference to spin coherent states which makes it possible to trace the passage from quantum mechanics to the limit of classical mechanics.

5.3. *Dynamics of quantum spin systems in the representation of spin coherent states. The integral approach*

As we have seen in the previous section, the application of spin coherent states allows one to develop naturally, from a common viewpoint, a convenient technique to describe quantum mechanical and thermodynamical properties of spin systems. Here we shall consider the dynamics of spin systems in the representation of spin coherent states. As in previous cases, the construction of an integral method will be discussed, which allows us to deal directly with averages of physical quantities avoiding the solution of the Schrödinger equation.

As was shown by Sinitsyn and Tsukernik [1982], for arbitrary nonlinear quantum systems described by variables of the coordinate and momentum types the averaging of the Heisenberg equations of motion over coherent states results in a closed linear equation for the averaged quantity. Since the diagonal matrix elements in the representation of coherent states completely determine an operator [Klauder and Sudarshan 1968], the time dependence of these elements provides a complete quantum description of the dynamics. In the limit $\hbar \to 0$ the quantum equations of motion change into the classical ones.

We shall see in this section how similar results are obtained for spin systems [Zaslavskii 1984a].

Consider the Heisenberg equations of motion for an arbitrary operator $\hat{g}(\boldsymbol{S})$ in the case of a time-independent Hamiltonian H,

$$\dot{\hat{g}} = (i/\hbar)(\hat{H}\hat{g} - \hat{g}\hat{H}) . \tag{5.27}$$

Let us average eq. (5.27) over a spin coherent state. Then, using relations (5.5), we obtain

$$\dot{g} = (i/\hbar)\hat{K}g , \qquad g = \langle \xi | \hat{g} | \xi \rangle , \qquad \hat{K} = H(\tilde{\boldsymbol{S}}) - \text{c.c.} \tag{5.28}$$

Since the quantity g goes not enter the operator $\hat{K}$, the difference between the solutions of eq. (5.28) for different g is determined only by the initial conditions. As follows from eq. (5.28), the study of the dynamics of an arbitrary quantum spin system is reduced to the solution of the Cauchy problem for a

partial differential equation of higher order, generally speaking, than one. Essentially, eq. (5.28) is closed and linear although the initial system is in general not linear.

Consider passing to the classical limit in eq. (5.28). Let $\hbar \to 0$, $S \to \infty$, so that the product $\hbar S = M = \text{const}$. Using relations (5.5) and taking into account that the classical Hamilton function H_{cl} should be expressed in terms of the components of the magnetization $M^i = \hbar S^i$, we get

$$\dot{g} = \{H_{\text{cl}}, g\}\,, \tag{5.29}$$

where $\{H_{\text{cl}}, g\}$ is the Poisson bracket,

$$\{H_{\text{cl}}, g\} = \sum_{i,k,l} \mathrm{e}_{ikl} M^i \frac{\partial H_{\text{cl}}}{\partial M^k} \frac{\partial g}{\partial M^l}\,,$$

and e_{ikl} is the unit antisymmetric pseudotensor. Since the operator $\{H_{\text{cl}}, \ldots\}$ contains derivatives with respect to the components of the magnetization (or ξ and ξ^*) of first order only, higher derivatives in eq. (5.28) have a purely quantum mechanical origin, as was established earlier for Bose systems [Sinitsyn and Tsukernik 1982].

Thus there is a classical limit for eq. (5.28) coinciding with the classical equations of motion (5.29). It should be stressed that this result was obtained due to averaging over a spin coherent state. The role of generalized coordinates is played by averages of the initial time values of the dynamical variables which can be expressed in terms of ξ and ξ^* [or of the angles θ and φ, see eq. (5.3)]. These sets of variables prove to be an essentially quantum mechanical generalization of Lagrange coordinates. In other words, it is just the use of Lagrange variables, not of Euler ones, that describes most adequately the passage from quantum mechanics to the classical limit.

The obtained results are relevant to averages of physical quantities. The use of spin coherent states also allows one to obtain a closed equation for the diagonal elements of a density matrix $\hat{\rho}$ averaging the Liouville equation. It differs from eq. (5.28) by a sign. A more essential difference is the following. In deriving eq. (5.28) the time independence of the Hamiltonian was used; as a result, its Heisenberg and Schrödinger representations coincide, and therefore the use of relations (5.5) is possible. Since the Hamiltonian from the very beginning enters the Liouville equation in the Schrödinger representation, a relevant equation for the diagonal elements of a density matrix in the representation of spin coherent states holds for both stationary and nonstationary systems [Zaslavskii 1984a].

Let us write the operator $\hat{K}$ of eq. (5.28) in terms of the variables ξ and ξ^*. To do this, we ought to mention that eq. (5.5) can be rewritten as

$$\tilde{S}_i = (1 + |\xi|^2)^{-2S} J_i (1 + |\xi|^2)^{2S}\,,$$

where the J_i are expressed only in terms of the variable ξ^* (a holomorphic representation),

$$J_+ = \partial/\partial\xi^*\,, \qquad J_- = 2S\xi^* - \xi^{*2}\,\partial/\partial\xi^*\,, \qquad J_z = S - \xi^*\,\partial/\partial\xi^*\,.$$

Making the substitution $\langle \xi | \hat{\rho} | \xi \rangle = (1 + |\xi|^2)^{-2S} F$ we come to the equation

$$\mathrm{i}\hbar \dot{F} = [H(\boldsymbol{J}) - \text{c.c.}]F\,, \tag{5.30}$$

which was obtained by Zaslavskii [1984a] and Tsuzuki [1986b].

Consider now specific examples. Let the system be an anisotropic paramagnet without an external magnetic field,

$$H = -DS_z^2 .$$

Write ξ as $\xi = \exp(\eta + i\varphi)$. Then the operator $\hat{K}$ reads

$$\hat{K} = -D\, i(\partial/\partial\eta + 2S \tanh\eta)\, \partial/\partial\varphi ,$$

and the problem of the dynamics can be solved exactly for an arbitrary initial condition. Then from eq. (5.28) one can find a function $f(t, \eta, \varphi)$ with initial condition

$$f|_{t=0} = \sum_n f_n(\eta)\, e^{in\varphi} . \tag{5.31}$$

The solution reads

$$f(t, \eta, \varphi) = \sum_n f_n(\eta + iDtn/\hbar)\left(\frac{\cosh(\eta + iDt/\hbar)}{\cosh\eta}\right)^{2S} e^{in\varphi} . \tag{5.32}$$

In a particular case, when $f|_{t=0} = -S\tanh\eta$, which is relevant to averaging of the component S_+ with respect to the state with spin projection S on the direction forming an angle θ with the z-axis [$\cos\theta = -\tanh\eta$, $\sin\theta = (\cosh\eta)^{-1}$], the solution (5.32) changes into formula (9) of Glazman [1979], where it was obtained in another way, viz.,

$$\langle S_+ \rangle = S\sin\theta\,[\cos(Dt/\hbar) - i\cos\theta\sin(Dt/\hbar)]^{2S-1} . \tag{5.33}$$

Consider now the temporal evolution of a uniaxial spin system in a transverse magnetic field [Zaslavskii et al. 1986],

$$H = -BS_z - DS_x^2 . \tag{5.34}$$

Assume anisotropy to be weak, $D \ll B/S$. In the absence of anisotropy, $D = 0$, the temporal behaviour of a spin in such a system is represented by precession around the z-axis and can be obtained from classical arguments. In this respect, allowing for anisotropy is of interest for finding out how quantum mechanical properties manifest themselves in nonlinear system dynamics.

In this case the equations of motion read

$$\begin{aligned}
&\dot{g} + \omega_0 \frac{\partial g}{\partial\varphi} = \frac{D}{\hbar}(2S\sin\theta\cos\varphi + \hat{l})\hat{m}g ,\\
&\hat{l} = \cos\varphi\cos\theta\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} ,\\
&\hat{m} = \sin\varphi\frac{\partial}{\partial\theta} + \cos\varphi\,\mathrm{cotan}\,\theta\frac{\partial}{\partial\varphi} ,\\
&\omega_0 = B/\hbar .
\end{aligned} \tag{5.35}$$

Let us confine ourselves to determining the average value of the component S_+, so that $g|_{t=0} = S\,e^{i\varphi}\sin\theta$. Then, in zeroth order in D

$$g^{(0)} = S\sin\theta\exp[i(\varphi - \omega_0 t)](\cos\tau + i\sin\tau\cos\theta)^{2S-1}, \quad \tau = Dt/\hbar\,. \tag{5.36}$$

Let us stress that already in the leading order in D the classical periodic dependence is modulated, having essentially a quantum mechanical origin. Therefore the spin motion turns out to be aperiodic, as should follow from the incommensurability of the eigenfrequencies of the Hamiltonian (5.34).

Note that, if one sets $D = 0$ in the leading order and tries to construct directly the perturbation series in D, this would lead to secular terms. Actually, this is a quantum mechanical generalization of the Bogolyubov–Krylov procedure [Nayfeh 1981].

An analogue of eq. (5.34) for Hamiltonian systems is the anharmonic oscillator with weak anharmonicity. The peculiarities of its temporal evolution and a more detailed discussion of the quantum mechanical generalization of this procedure were considered by Zaslavskii et al. [1986].

It is of interest that the modulational part of the temporal dependence (5.36), which describes the spin behaviour in a strong (compared with the anisotropy) magnetic field, is analogous to the spin dynamics with the same initial condition but in the absence of the field (5.32) [Glazman 1979; Zaslavskii 1983].

It is apparent from eq. (5.36), in the leading order in D and in a reference frame rotating with angular velocity ω_0, that the spin oscillates in a purely quantum mechanical way. Besides, in the interval $0 \le \tau < \pi$ each of the transverse spin components in this reference frame becomes zero precisely $2S - 1$ times regardless of the θ value. In the limit $\theta \to \pi/2$, in which the quantum mechanical properties of the system are most pronounced, all the zeros merge into only one, which is thus degenerate with multiplicity $2S - 1$.

Next let us present a generalization of eq. (5.36) for an arbitrary function of spin operators to the case of biaxial anistropy, for which the Hamiltonian differs from eq. (5.34) in the additional term $-ES_z^2/2$. Introduce the variable η according to the equality $\cos\theta = -\tanh\eta$, as was done above in deriving eq. (5.32). Then for an initial condition of the type (5.31) we obtain an expression which differs from eq. (5.32) by the substitutions $\varphi \to \varphi - \omega_0 t$, $D \to \frac{1}{2}(D - E)$, $t \to -t$. It is apparent from this, in particular, that there is no modulation for the longitudinal component $\langle S_z \rangle$. It is also absent (in this approximation) for equal constants of anisotropy, $D = E$.

The analysis performed here (see also [Zaslavskii et al. 1986; Berman et al. 1981; Zaslavskii 1984]) demonstrates that even for a quantum system that is maximally "close" to a classical one (because the initial state is chosen to be coherent) the presence of a weak nonlinearity results in a qualitative difference in the behaviour of the quantum and the classical systems. Although in this case the temporal evolution is related to the nonstationarity of the initial state, one may assume that the relevant methods and results will be also useful in more complicated situations, for instance, in studying periodic effects in nonlinear systems.

6. Summary and outlook

The approach considered in this review (as a rule, related in some way to the spin coherent state representation) has allowed us to describe a whole series of systems of a different nature from a united viewpoint. This concerns both variation in the physical objects and regions which the developed

methods can be attributed to (quantum theory of magnetism, nuclear physics, theory of the interaction of light with matter, etc.) and variation in the structures and models themselves. The latter can be united using the effective potential method (anisotropic paramagnet, Dicke model, Heisenberg model, connected anharmonic oscillators, etc.). Therefore the correspondence between coordinate systems and different systems having a discrete nature turns out to be simultaneously a means to investigate potential models and, on the other hand, a convenient technique to study physical properties of spin, pseudospin, etc. systems using the convenient concept of a particle moving in a potential.

Let us also point to a series of integral methods (compare Ulyanov [1982]) with which both the energy quantization rules were derived and the dynamics of spin systems was studied using spin coherent states, without solving the Schrödinger equation, thus avoiding the stage of finding a wave function.

Without reproducing the specific results presented above, we would like to concentrate on the perspectives. We stress that the issues considered in this review (first, the method of effective fields and the study of quasi-exactly solvable models) actually refer to a field that emerged very recently and is extensively developed at present. Therefore it seems reasonable to mention both the aspects not presented in this review and possible directions of further research.

One of the traditional problems of quantum mechanics is the investigation of the analytical properties of the energy as a function of the parameters of the potential. In application to the anharmonic oscillator this problem was studied earlier by Bender and Wu [1969] and Simon [1970] using approximate methods. It turned out that for a sextic anharmonic oscillator (see section 3.5) for a certain relation between the coefficients one can find explicit expressions for the energy levels of the low-lying states. This has allowed progress in understanding the analytical properties of different types of models in quantum mechanics [Turbiner and Ushveridze 1987; Turbiner 1988a, b, c] falling in exactly solvable, exactly nonsolvable and quasi-exactly solvable classes.

After this review was completed, we became aware of some recent papers close to the subject of our work. It is worth noting the review by Ushveridze [1989], which is mainly of a mathematical nature and deals with an approach different from ours to study quasi-exactly solvable models. In particular, the equivalence was pointed out therein between problems of quantum mechanics, specifically, of the quantum theory of perfectly integrable systems, and of many-particle Coulomb problems of classical physics.

This analogy turned out to be clear in the discussion by Shifman [1988a] of the ways in which the class of quasi-exactly solvable problems can be expanded.

An interesting question which requires a separate treatment is the connection between quasi-solvable problems and supersymmetric quantum mechanics, which was shown to enable us to expand this class [Shifman 1988b]. The sextic oscillator has been treated in this framework by Roy et al. [1989]. The properties of the Witten index for sypersymmetric quantum models which are soluble both on the line and on the circle and include the case of the Lamé equation, were discussed by Braden and Macfarlane [1985].

The effective spin Hamiltonian for this equation was recently rediscovered by Postell and Uzer [1990] in the context of the quantum theory of action–angle variables [Carruthers and Nieto 1968; Augustin and Rabitz 1979; Augustin et al. 1980]. The accuracy of the quasiclassical rules of quantization for the Lamé equation was discussed by Pajunen [1985].

The possibility to find exact solutions for a sextic anharmonic oscillator was pointed out by Dutta and Willey [1988] and Singh et al. [1990].

It is worth noting two recent papers devoted to approaches of spin in quantum mechanics different from ours. Stone [1989] discussed the quantum mechanical basis of the well-known fact that Bohr–

Sommerfeld quantization is exact for a spin in a magnetic field. He showed this result to be connected with the existence of a hidden suppersymmetry. The semiclassical quantum mechanical interpretation of the Weyl character formula for compact, semisimple Lie groups was also discussed. In a paper by Varilly and Gracia-Bondia [1989] the phase space approach to spin is developed in the spirit of the Moyal representation. Developing ideas of Stratonovich [1956], the authors suggest the Moyal representation for spin in a fully explicit mathematical setting.

We considered the dynamics of nonlinear spin systems of a general type in terms of spin coherent states, which is similar to the evolution of the quantum mechanical anharmonic oscillator in terms of ordinary coherent states. The evolution of an anharmonic oscillator of a special type was considered by Gerry [1987] and Bužek [1989] with the help of Holstein–Primakoff SU(1, 1) coherent states. The corresponding model describes the interaction of squeezed light with a nonabsorbing nonlinear medium.

Let us now briefly outline some unsolved problems on the matter considered. Of interest is the explicit generation of new quasi-exactly solvable models from ones already known [Razavy and Pimpale 1988; Jatkar et al. 1989] using the transformations of Darboux and Gelfand–Levitan [Gelfand and Levitan 1955; Chadan and Sabatier 1977; Abrahams and Moses 1980].

The problem was posed by Zaslavskii and Ulyanov [1984, 1987] and Turbiner [1988c] to investigate the possibility of the existence of quasi-exactly solvable models whose structure is not based on the SL(2) algebra. The corresponding example is discussed by Jatkar et al. [1989].

It seems necessary to find a rigorous mathematical proof of the structure transformations in the energy spectrum of potentials considered in section 3.4 (they were discovered using numerical methods); it may turn out to be a generalization of finite-band potential theory.

In the paper by Shifman and Turbiner [1989] the generalization to the two-dimensional case was performed. In so doing, the Schrödinger equation was obtained in curved Riemannian space.

It would be especially interesting to try to construct the effective potential for such systems of physical interest as the Heisenberg model (which was done in section 4.2 approximately and in section 3.5 exactly, but only for two interacting spins). A similar problem arises for the three-level generalization of the Lipkin–Meshkov–Glick model [Meredith et al. 1988] in connection with studies of quantum chaos.

Speaking about applications, let us first pay attention to the tunnelling problem for spin systems with dissipation taken into account. One may suppose that the effective potential method might be useful here.

It would also be interesting to find a possibility to describe continuous spin systems in terms of an effective potential (in particular, applications related to tunnelling).

It would be quite useful to formulate energy quantization rules of the Bohr–Sommerfeld type with allowance for quantum corrections for systems described on the basis of the SU(1, 1) algebra (and more complicated cases) with the aid of the nonfunctional approach described in section 5.2 and of generalized coherent states, as was done in section 5 for spin systems.

The authors hope that this review will facilitate new studies and stimulate the publication of new reviews in the considered field which is rich with both unexpected mathematical results and a variety of physical applications.

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