Tunnelling series in terms of perturbation theory for quantum spin systems

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Considered is quantum tunnelling in anisotropic spin systems in a magnetic field perpendicular to the anisotropy axis. In the domain of small field the problem of calculating tunnelling splitting of energy levels is reduced to constructing the perturbation series with degeneracy, the order of degeneracy being proportional to a spin value. Partial summation of this series taking into account "dangerous terms" with small denominators is performed and the value of tunnelling splitting is calculated with allowance for the first correction with respect to a magnetic field.

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Tunnelling splitting of energy levels and the appearance of gaps in the energy spectrum of a quantum system is connected with breaking the symmetry of an unperturbed system by perturbation removing degeneracy. Usually, this effect is realized in quantum mechanics in two typical situations. The first one consists in that the Hamiltonian can be represented in the form $H = H_0 + V$ where $H_0$ is the unperturbed Hamiltonian and $V$ is perturbation, so correction to energy levels can be calculated with the help of some version of the perturbation theory. Another situation is tunnelling splitting of energy levels for a particle moving in a symmetric double well due to tunnelling penetration into a classically forbidden region. In that case the tunnelling splitting can be found by means of one of quasiclassical methods (WKB, instanton calculus, etc.). Although the physical reason - removing degeneracy - is the same in both cases, it is described in terms of essentially different languages regions of applicability of which, generally speaking, do not match.
It turns out, however, that there exists a whole class of physically interesting systems for which both approaches can be combined - anisotropic spin systems whose Hamiltonian is a quadratic-linear combination of spin operators. Their energy spectrum admits rigorous description in terms of an effective potential [1]: energy levels of a spin system coincide with $2S + 1$ low-lying levels for a particle moving in a potential field of a certain form. If such a spin system is of the easy-type, for a sufficiently small field the corresponding potential has the form of a double well typical of tunnelling effects, so the energy splitting can be obtained, for example, with the help of instanton formulas [1], [2] accuracy of which grows as a magnetic field decreases and the spin value increases. On the other hand, in the domain of small fields the perturbation theory can be applied. Thus, for sufficiently small magnetic fields and $S \gg 1$ both approaches match.

The nontrivial peculiarly of the perturbation theory in such a situation consists in that the order of degeneracy is proportional to the spin value [3]. As the quantity $S$ plays the role of the inverse Planck constant $\hbar$, it turns out that the degree of degeneracy tends to infinity in the quasiclassical limit. In so doing, the terms like $B^{2S}$ appear in the perturbation series which are nonanalytic with respect to $S^{-1}$ in the limit $S \rightarrow \infty$ that in itself testifies that, although calculations are carried out on the basis of perturbation theory, the effect in fact admits the tunnel interpretation.

In the leading order of perturbation theory the result of the calculation of tunnelling splitting has been reported in [4] (without detailed derivation) and, independently, in [1] where a consistent derivation of the formulas for energy splitting was suggested. This derivation was not direct application of standard formulas of the perturbation theory form textbooks and required careful singling out and summing all ”dangerous” terms. In the present paper we perform the next step and calculate the first non-vanishing correction to the tunnelling splitting for an arbitrary value of a spin. The approach developed in [1] and the present paper is of systematic character that enables one to construct the series with respect to a magnetic field value including high-order corrections. In this sense the calculation of tunnelling rate is reduced to summing up the perturbation theory series with a given accuracy.
In recent years the interest to the nature of quantum tunnelling in spin systems of different nature sharply increased. It concerns the crossover between quantum and thermal domains \[\text{[5]}\], tunnelling in small ferromagnet particles \[\text{[6]}\], many-spin molecules \[\text{[7]}\], etc. Therefore, formulae for the tunnelling splitting obtained below can be of interest not only from a viewpoint of general methods of quantum theory but for description of concrete physical systems observable in experiments.

Let us consider the system described by the Hamiltonian

\[ H = -S^2_z - BS_x \]  

(1)

Here \( S_i \) are the operator of a corresponding spin component, \( B \) is a magnetic field. Since the first terms enters (1) with a negative sign, the system has an easy axis \( z \). In the absence of a magnetic field all energy levels, except the one with \( S_z = 0 \) in the case of an integer \( S \), are two-fold degenerate. A magnetic fields removes this degeneracy. The problem is to calculate the energy splitting due to quantum tunnelling with the first correction in \( B \) taken into account when \( B \to 0 \).

Consider the Brillouin-Wigner perturbation series

\[ E = \varepsilon_\sigma + \frac{V_{\sigma,\sigma-1}^2}{\alpha_{\sigma-1}} + \frac{V_{\sigma,\sigma+1}^2}{\alpha_{\sigma+1}} + \ldots \]  

(2)

where \( \varepsilon_\sigma = -\sigma^2 \) corresponds to the unperturbed level with a \( z \)-projection of spin equal to \( \sigma \), \( \alpha_\sigma = E - \varepsilon_\sigma \), the perturbation \( V = -BS_z \) and we took into account that diagonal matrix elements of perturbation are equal to zero. In order to determine \( \Delta E_\sigma \) correctly, one needs to take into account explicitly the role of small denominators in "dangerous" terms of the perturbation series by performing a partial summation of (2). Following \[\text{[1]}\], we sketch this procedure below. Consider, for simplicity, the splitting for the ground energy level \( \Delta E_0 \).

The leading "dangerous" terms \( f \) reads

\[ f = \frac{(V_{S,S-1}V_{S-1,S-2} \ldots V_{S+S-1,S})^2}{((E - \varepsilon_{S-1})(E - \varepsilon_{S-2}) \ldots (E - \varepsilon_{S+S-1}))^2}(E - \varepsilon_{-S})^{-1} \]  

(3)

If we introduce a sequence of points on a number axis from \( S \) to \(-S\) corresponding to different values of \( \sigma \), 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 back 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 values of σ). 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 leads to the following for m of the last retained term in the perturbation series:

\[ f \rightarrow \tilde{f} = f(1 + r + r^2 + ...) = f(1 - r)^{-1}, \quad r = (E - \varepsilon_S)^{-1} \chi, \quad \chi = \frac{V_{-S,s+1}V_{-S+1,-S} + ...}{E - \varepsilon_{-S+1}} \]

(4)

The factor \( \chi \) has the same form as the initial perturbation series (2) that allows one to construct a simple equation with respect to \( E \):

\[ (E - \varepsilon_\sigma - \frac{V_{S,S-1}^2}{E - \varepsilon_{S-1}} - \frac{V_{S,S+1}^2}{E - \varepsilon_{S+1}} + ...)^2 = g_\sigma^2, \quad g_\sigma = \frac{V_{S,S-1}V_{S-1,S-2}...V_{S+1,-S}}{(E - \varepsilon_{S-1})(E - \varepsilon_{S-2})...(E - \varepsilon_{-S+1})} \]

(5)

Generalization to other levels is straightforward and the result reads

\[ (E - \varepsilon_\sigma - \frac{V_{S,\sigma-1}^2}{E - \varepsilon_{\sigma-1}} - \frac{V_{\sigma,\sigma+1}^2}{E - \varepsilon_{\sigma+1}} + ...)^2 = g_\sigma^2, \quad g_\sigma = \frac{\Pi_{k=0}^{2\sigma-1} V_{\sigma-k,\sigma-k-1}}{\Pi_{k=1}^{2\sigma-1} \alpha_{\sigma-k}} \]

(6)

The differences of the signs corresponds to the level splitting (the remaining terms coincide, making no contribution to the splitting). Taking advantage of the explicit form of the matrix elements \( V_{\sigma,\sigma'} \) we get

\[ \Delta^{(0)}E_\sigma = 2g_\sigma = 2\left(\frac{B}{2}\right)^{2\sigma} \frac{(\sigma + S)!}{(S - \sigma)!(2\sigma - 1)!} \]

in accordance with [4], [1] where \( \sigma = S - n \), \( n \) is the number of the unperturbed level.

The first correction to (7) stems from three origins. First, the value of \( g_\sigma \) in (8) acquires the correction due to field dependence of levels \( E_\sigma \). Second, the correction appears due to \( E_\sigma \) which enter denominators in terms containing \( V^2 \) in the left hand side of (8). Third, the correction arises because of the next order terms in the perturbation series itself which change
the structure of \( g_\sigma \). Let us write down the total fractional correction as 
\[
\xi \equiv \frac{\Delta E_\sigma}{\Delta E_\sigma} \equiv \xi_1 + \xi_2 + \xi_3
\]
and calculate each term separately.

The first term \( \xi_1 = \Pi_{k=1}^{2\sigma-1} \frac{E_\sigma^{(0)} - \varepsilon_\sigma - k}{(E_\sigma^{(0)} - \varepsilon_\sigma) - k} \). Substituting into this formula the explicit expression for unperturbed levels \( E_\sigma^{(0)} = -\sigma^2 \) and take into account the second order correction to \( E \) which can be easily found from the standard perturbation theory we obtain \( n = S - \sigma \)

\[
\xi_1 = \frac{-B^2 \left[ n^2 - 2Sn + S(2S + 1) \right]}{(2S - 2n)(2S - 2n + 1)^2 - 1} \sum_{k=1}^{2S-2n-1} k^{-1}
\]

(8)

The second type contribution to the correction can be found directly from the Brillouin-Wigner perturbation series by elementary methods:

\[
\xi_2 = \frac{-B^2}{4} \left\{ \frac{(n + 1)(2S - n)}{(2S - 2n - 1)^2} + \frac{n(2S - n + 1)}{(2S - 2n + 1)^2} \right\}
\]

(9)

The calculation of \( \xi_3 \) is the nontrivial and rather cumbersome part of computations. This quantity is connected with the correction to the perturbation theory itself which is to be now cut off at terms of the order \( B^{2S+2} \). According to [1], a typical term of the perturbation theory series arises as follows. It is necessary to take the segment \([-\sigma, \sigma]\) and allow for all possible paths of the transition between these two points provided each an intermediate point on each path is being passed two times (to and fro). The main corrections to these terms arise if the transition from a given point to a next one contains one extra jump to and one - fro (delay and ”marking time”). Summing up over all possible points - origins of extra jumps to and fro - we obtain

\[
\xi_3 = \sum_{k=2}^{2S-1} \frac{V_{\sigma-k,\sigma-k+1}^2}{\alpha_{\sigma-k} \alpha_{\sigma-k+1}}
\]

(10)

Summing up all three contributions we find, after direct but somewhat lengthy calculations, the final expression which proves to be surprisingly simple:

\[
\xi = 1 - B^2 \gamma,
\]

(11)

\[
\gamma = \frac{(2S + 1)^2(\sigma + 1)}{2(2\sigma - 1)^2(2\sigma + 1)^2}
\]

Thus, for an arbitrary energy gap (except the highest one in the case of semi-integer \( S \)) we get
\[ \Delta E_n = \frac{(2S-n)!}{2^{2S-2n-1}n!(2S-2n-1)!}B^{2S-2n}[1 - \frac{(2S+1)^2(S-n+1)}{2(2S-2n-1)^2(2S-2n+1)^2}] \]  

(12)

This formula is supplemented for semi-integer \( S \) by the expression for the highest gap:

\[ \Delta E_{S-1/2} = (S + \frac{1}{2})B[1 - \frac{1}{16}(S + \frac{3}{2})(S - \frac{1}{2})B^2] \]  

(13)

The obtained formulae, as was mentioned above, are valid when \( B \to 0 \). However, the presence of the correction term in (12) and (13) aids to make the area of applicability of these formulas more precise. First of all, the correction gives a qualitative notion about the approximation: it is seen that without account for such a correction the result is overstated. 

Further, the quantitative role of the correction turns out two-fold.

First, it enables us to estimate the accuracy of the first approximation. Let us restrict ourselves by remarks concerning the ground gap \( (S > 1/2) \)

\[ \Delta E_0 = \frac{S^2}{2^{2S-3}(2S)!}B^{2S}[1 - \frac{(S + 1)}{2(2S - 1)^2}] \]  

(14)

It is seen from this formula that in the case \( S \gg 1 \), with the correction neglected, the fractional error is \( B^2/8S \). That means that even for \( B = \sqrt{S} \) the computation of the ground gap gives the error approximately 10\% while in the case \( B = 1 \) it proves to be very small, being of the order \( 0.1/S \).

Second, the allowance for the correction essential increases the accuracy of computations. Thus, even for so large values of a magnetic field as \( \sqrt{S} \) can be thought of to be, taking into account the correction enables one to make the fractional error one order smaller.

It is worth noting that while computing energy gaps numerically even for moderately large values of \( S \) one is led to take into account very big number of digits that can be achieved only by modern computer computation systems. For example, in the case \( B = 1, S = 10 \) the gap has the order \( 10^{-20} \) while for \( S = 50 \) it is of the order \( 10^{-200} \).

Either the main term or the correction in (14) are in agreement with the instanton approach [1] but for \( S \gg 1 \). Meanwhile, it is worth stressing that formulae (12)-(13) are applicable for all values of \( S \) and embrace all the gaps.
In the case of an easy-plane spin system, i.e. a system with a Hamiltonian \( H = +S_z^2 - BS_x \), the energy spectrum of which differs from that of the easy-axis type by the interchange of the sign of energy. Therefore, formulae for gaps remains valid provided they are renumbered, so that the lowest gap becomes the highest and vice versa. As far as the effective potential is concerned, in this case we have the model of a periodic potential energy in which the energy levels of a spin system coincide with the corresponding edges of energy bands (\[\text{[1]}\]).

The elaborated approach describes quantum tunnelling in terms of the perturbation theory and enables one, in principle, to construct the energy level splitting as a series with respect to \( B \) with any given accuracy.

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