

# Simple Calculation of Quantum Spin Tunneling Effects

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## Abstract

The level splitting formulae much discussed in the study of spin tunneling in macroscopic ferromagnetic particles and previously derived only by complicated pseudoparticle methods for the ground state, are derived from those of eigenvalues of periodic equations and extended to excited states.

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In recent years the tunneling of quantum spins and the possibility of its observation in macroscopic ferro- or antiferromagnetic particles has attracted considerable interest as the rapidly expanding literature in the field demonstrates [1, 2]. The principal idea is that in such particles of mesoscopic size the electronic spins can form an aligned magnetic state which can assume several directions so that quantum mechanics suggests the possibility to lift this degeneracy by tunneling from one direction to another. This tunneling effect and its possible suppression in half-integer-spin particles (with or without applied magnetic fields) has been explored in numerous investigations [3, 4, 5]. In most of these the first step is the conversion of the discrete spin system into a continuous one [6, 7] by transforming spin operators to canonical operators  $\hat{p}, \hat{q}$  satisfying the quantisation relation

$$[\hat{q}, \hat{p}] = \frac{i}{s}$$

where  $s$  is the spin quantum number of the particle. The calculation of the basic semiclassical Hamiltonian is quite involved and can be found in the literature [8, 9], and will therefore not be repeated here. Once the approximate effective quantum hamiltonian has been constructed, the next step is usually to proceed to the appropriate Lagrangian and then to the application of the path-integral method. Here, however, a problem arises. Since the effective Hamiltonian is that of a particle with position- or field-dependent mass (see below), the path-integral method must start from the phase-space path-integral, as pointed out long ago [10]. The resulting evaluation of the path-integral by expansion about a classical configuration [8, 9, 11, 12] which itself is already a complicated expression in many cases (involving sometimes elliptic functions) is so complicated that one would like to have a verification of the resulting formulae, at least in some limiting cases, although, no doubt, the pseudoparticle methods applied to these theories are of considerable interest in themselves. Nonetheless, particularly experimentalists interested in spin tunneling phenomena might welcome a more straightforward derivation of the relevant level splitting formulae. Our objective here is therefore to point out that in certain cases such a simpler verification is possible by reference to some standard (though possibly not so well-known) quantum mechanical problems, and yields even the splitting of the appropriate excited state levels (a definite advantage over the instanton method). In the following we therefore demonstrate that in the case without an applied magnetic field the level splitting formulae for the ground state as well as excited states can be obtained from those of Schrödinger equations with periodic

boundary conditions. In the limit of vanishing position- or field-dependence of the effective mass the comparison equation is the Mathieu equation, and in the case with position-dependence it is the (even less well-known) Lamé equation. In both cases the results are easily extendable to excited states and the range of validity of the results can be clearly inferred from the validity of the asymptotic solutions of these equations. The results, which verify previous path-integral calculations, also demonstrate that the field dependence of the effective mass provides only a minor change. We expect that the derivation given here may be helpful also in the verification of the results of some other tunneling model theories.

The Hamiltonian of the theory describing the ferromagnetic particle is given by

$$\hat{H} = K_1 \hat{S}_z^2 - K_2 \hat{S}_x^2$$

in terms of spin operators  $\hat{S}_x, \hat{S}_z$  and  $K_1 > K_2 > 0$ , the two contributions describing  $XOY$ -easy plane anisotropy with easy axis along the  $x$  direction [3]. As mentioned above the spin operators are transformed to canonical operators  $\hat{p}, \hat{\phi}$  [6] with  $\hat{S}_z = s\hat{p}$  and  $[\hat{\phi}, \hat{p}] = \frac{i}{s}$ . One then obtains an effective Hamiltonian which has been used in the following form in the literature [8, 9, 11, 12]

$$\hat{H} = s^2 \frac{\hat{p}^2}{2m(\hat{\phi})} + V(\hat{\phi}) \quad (1)$$

where

$$m(\phi) = \frac{1}{2K_1(1 - \lambda \sin^2 \phi)}, \quad V(\phi) = K_2 s^2 \sin^2 \phi \quad (2)$$

and  $-\pi \leq \phi \leq \pi$ . We consider first the case of constant mass, i.e.  $\lambda = 0$ , although in actual fact [8, 9]  $\lambda = K_2/K_1$ . The problem is to determine the splitting of asymptotically degenerate energy levels of the Schrödinger equation  $\hat{H}\psi = E\psi$  for the given periodic potential. Setting

$$h^2 = \frac{s^2 K_2}{4K_1}, \Lambda = \frac{E - s^2 K_2}{K_1} + 2h^2, b = \frac{K_1}{K_2} \quad (3)$$

the Schrödinger equation becomes the Mathieu equation

$$\psi''(\phi) + (\Lambda - 2h^2 \cos 2\phi) \psi = 0 \quad (4)$$

The tunneling splitting of the eigenvalues  $\Lambda$  of this equation (which is twice the shift of a single level) has been derived in the literature [13] from periodic

boundary conditions. In terms of the quantum number  $q_0 = 2n + 1, n = 0, 1, 2, \dots$  the dominant term can be written

$$\Delta_{q_0}\Lambda = \frac{2(16h)^{\frac{1}{2}q_0+1}e^{-4h}}{(8\pi)^{\frac{1}{2}}[\frac{1}{2}(q_0-1)]!} \left(1 + O\left(\frac{1}{h}\right)\right) \quad (5)$$

For the ground state (i.e.  $q_0 = 1$ ) this yields the level splitting of our original problem here, i.e.

$$\Delta_1 E = K_1 \Delta_1 \Lambda = \frac{16K_1}{\sqrt{\pi}} \left(\frac{s}{\sqrt{b}}\right)^{\frac{3}{2}} e^{-2\left(\frac{s}{\sqrt{b}}\right)} \quad (6)$$

Comparing this with the result of [8] in the same limit (i.e. for no applied field and the parameter  $a \rightarrow 0$ ) in [8]) one obtains the same result except that in [8] the exponential factor is missing. The exponential factor is crucial evidence of the nonperturbative nature of the calculation (in the calculations underlying (5) the effect of boundary conditions), and its argument usually represents the euclidean action of the appropriate instanton. The exponential factor is missed in [8], presumably as a consequence of the approximation considered which then is the leading approximation of that under discussion and is therefore indicative of the approximation there employed. This also shows the conditions on the parameters under which the result is valid. The parameter  $h^2$  of eq.(3) has to be large, and the result is the dominant contribution of an asymptotic expansion in descending powers of  $h^2$ . This condition implies that  $s^2 \gg 4b$ , as also realised in [8]. An additional advantage of the Schrödinger equation method given here is that it yields immediately also the level splitting for excited states, which cannot be obtained with the usual instanton method, but instead requires the corresponding consideration of nonvacuum (or periodic) instantons or some other method as in [12].

We now want to take the  $\phi$ -dependence of the effective mass  $m(\phi)$  into account. The expression itself in eq.(2) is reminiscent of an elliptic expression. This suggests searching for an analogy with an elliptic equation like the Lamé equation. We set  $x = \sin \phi$  and  $\psi = (1 - x^2)^{-\frac{1}{4}}\Phi$ . We then expand the coefficient of  $\Phi$  in the resulting equation in ascending powers of  $x$  and obtain an equation which we can write (with  $-\frac{2\lambda x^2}{4} \equiv -\frac{6\lambda x^2}{4} + \lambda x^2$ )

$$(1 - x^2)(1 - \lambda x^2)\Phi'' + \left\{\frac{1}{4} \left[2 + 2\lambda + x^2(3 - 6\lambda) + x^4(3 - 3\lambda)\right]\right\}$$

$$+ \left( \frac{(E - s^2 K_2)}{K_1} - \frac{\lambda}{2} \right) - \left( \frac{s^4 K_2}{\lambda K_1} - 1 \right) \lambda x^2 + O(x^6, \lambda^2) \Big\} \Phi = 0 \quad (7)$$

The Lamé equation is best known in the form [14]

$$w'' + \{ \Lambda - n(n+1)k^2 sn^2 z \} w = 0 \quad (8)$$

The eigenvalues  $\Lambda$  and eigenfunctions  $w$  of the equation with periodic boundary conditions can be found in the literature [14]. The level splitting analogous to that of the Mathieu equation is not so well-known but also available in the literature [15]. In fact, under certain conditions the Lamé equation reduces to the Mathieu equation. In eq.(8)  $n$  is an integer in the case of Lamé polynomials, and  $k$  is the elliptic modulus of the Jacobian elliptic functions. The quantity  $\Lambda$  is the eigenvalue. To a good approximation we can convert eq.(8) into one similar to eq.(7). To this end we set  $t = snz$  and  $w = [(1-t^2)(1-k^2t^2)]^{-\frac{1}{4}} \Xi$ . The equation for  $\Xi$  is then

$$(1-t^2)(1-k^2t^2)\Xi'' + \left\{ \frac{1}{4} [2 + 2k^2 + t^2(3-6k^2) + t^4(3-3k^2)] \right. \\ \left. + \Lambda - n(n+1)k^2t^2 + O(k^4, t^6) \right\} \Xi = 0 \quad (9)$$

Comparing eq.(7) with eq.(9) we can identify the following quantities

$$\lambda \equiv k^2, \frac{(E - s^2 K_2)}{K_1} - \frac{\lambda}{2} \equiv \Lambda, \kappa^2 \equiv \left( \frac{s^4 K_2}{\lambda K_1} - 1 \right) \lambda \quad (10)$$

The level splitting of the eigenvalue  $\Lambda$  of the Lamé equation is known to be in leading order of  $\kappa^2 = n(n+1)k^2$  [15]

$$\Delta \Lambda_{q_0} = 4\kappa \left( \frac{2}{\pi} \right)^{\frac{1}{2}} \left( \frac{1+k}{1-k} \right)^{-\frac{\kappa}{k}} \frac{\left( \frac{8\kappa}{1-k^2} \right)^{\frac{1}{2}q_0}}{[\frac{1}{2}(q_0-1)]!} \left( 1 + O\left(\frac{1}{\kappa}\right) \right) \quad (11)$$

where for small values of  $k$

$$\ln \left( \frac{1+k}{1-k} \right) = 2k + \frac{2}{3}k^3 + O(k^5).$$

In the case of the ground state ( $q_0 = 1$ ) eq.(10) implies the splitting of the Schrödinger eigenvalue  $E$  given by

$$\Delta E_1 = \frac{16K_1}{\sqrt{\pi}} \left( \frac{s}{\sqrt{b}} \right)^{\frac{3}{2}} \frac{e^{-\frac{s}{\sqrt{b}}(2+\frac{2}{3}k^2)}}{\sqrt{1-k^2}} \left( 1 + O\left(\frac{1+k^2}{\kappa}\right) \right) \quad (12)$$

We compare this result with that given in [9] (there eq. (9a)) and calculated with the help of a complicated instanton method. For the comparison we have to set in our result  $k^2 = \frac{1}{b}$ , so that eq.(12) becomes

$$\Delta E_1 = \frac{16K_1}{\sqrt{\pi}} \left( \frac{s}{\sqrt{b}} \right)^{\frac{3}{2}} \left( 1 + \frac{1}{2b} \right) e^{-\frac{s}{\sqrt{b}}(2+\frac{2}{3b})} \quad (13)$$

The corresponding expression obtained in the literature [9] by the instanton method is with  $B = K_1$

$$\begin{aligned} \Delta E_1 &= \frac{16B}{\sqrt{\pi}} \left( \frac{s}{\sqrt{b}} \right)^{\frac{3}{2}} \left( 1 + \frac{1}{b} \right)^{\frac{3}{4}} \left[ \left( 1 + \frac{1}{b} \right)^{\frac{1}{2}} - \left( \frac{1}{b} \right)^{\frac{1}{2}} \right]^{2s+1} \\ &= \frac{16B}{\sqrt{\pi}} \left( \frac{s}{\sqrt{b}} \right)^{\frac{3}{2}} \left( 1 + \frac{3}{4b} \right) e^{-\frac{s}{\sqrt{b}}(2-\frac{1}{3b})} \end{aligned} \quad (14)$$

We observe that except for small differences in the coefficients of the effects of the field dependence of the effective mass, the expressions obtained by these totally different methods agree with one another. We interpret the small differences in the coefficients as due to unavoidable and somewhat different approximations in the two methods. Our procedure here extends the previous results in several ways. First, one can clearly see that the result is the dominant contribution of an asymptotic expansion in descending powers of  $\kappa = \frac{s^2}{b}$ . This is therefore the parameter which is assumed to be large, in agreement with the condition on  $h^2$  above and experimentally relevant values. Secondly, apart from the simple reference to the result in the literature, this Schrödinger method yields also immediately the level splitting of excited states which are much more difficult to obtain with a pseudoparticle method. Since these are easily obtained from the cited formulae above we do not write them down in detail for the problem under discussion.

Concluding we can say that the level splitting formulae, which have been much discussed in connection with spin tunneling in macroscopic particles

but have previously been derived only by complicated pseudoparticle path-integral methods can readily be obtained in equivalently good approximation from the level splitting of eigenvalues of periodic equations, which admittedly are not so well known but have been studied extensively in the literature. This simpler way of deriving these formulae should appeal particularly to experimentalists.

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