KL–TH 97/5

Calculation of Spin Tunneling Effects in the Presence of an Applied Magnetic Field

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Abstract

The tunneling splitting of the energy levels of a ferromagnetic particle in the presence of an applied magnetic field – previously derived only for the ground state with the path integral method – is obtained in a simple way from Schrödinger theory. The origin of the factors entering the result is clearly understood, in particular the effect of the asymmetry of the barriers of the potential. The method should appeal particularly to experimentalists searching for evidence of macroscopic spin tunneling.

PACS numbers:11.15KC, 73.40GK, 75.60JP, 03.65Db

In spite of early speculation[1] that the one loop approximation of a path integral calculation in quantum mechanics would not yield exactly the same result as a WKB semiclassical calculation, it is now generally agreed – and has indeed been verified by application to important examples – that the two approaches yield exactly the same result in the approximation of correct linear matching of WKB solutions across turning points. Thus with this proviso the latter method was shown [2] to lead to the same level shifts in the cases of the double–well and periodic potentials as the path integral method with expansion around an instanton. The effect of the nonlinearity which gives rise to instanton or other classical solitonic configurations arises in Schrödinger quantum mechanics through the boundary conditions imposed on the perturbatively calculated wave functions. It is these boundary conditions therefore which generate the nonperturbative effects characteristic also of tunneling.

Once the Hamiltonian of a theory with tunneling effects has been established, it is still a long way to obtain the level shift or decay rate with the path integral method. Such calculations are very instructive, particularly as models for more complicated field theoretical contexts, but can lack transparency in other contexts where a confrontation with experiments is anticipated. Thus recently long and complicated instanton path integral calculations [3, 4, 5, 6, 7, 8, 9, 10, 11] were performed in order to derive the tunneling splitting of the ground state of a magnetic particle in a crystal field with or without an applied magnetic field. This is a case which is of considerable experimental interest since the tunneling rate should be directly experimentally measurable in resonance experiments[11]. It seems it is not so well known that the calculation of such tunneling effects can also be performed in the context of Schrödinger theory with appropriately chosen (in this case periodic) boundary conditions, and in fact much more directly so by comparison with established cases as demonstratred recently in the case with no applied magnetic field[12]. On the basis of our experience with both types of methods (for path integral calculations see also refs.[13, 14, 15]), we expect that any calculation which is manageable in the path integral method can also be dealt with in Schrödinger theory and vice versa. In fact, the latter even has certain advantages in yielding with equivalent ease (or complexity) the corresponding results for excited states whereas in the path integral method this would necessitate the consideration of periodic or nonvacuum instantons[14, 15] which implies a further degree of considerable calculational complication.

Quantum spin tunneling (or more generally tunneling for internal degrees of freedom) has only recently been realised to be a fascinating quantum mechanical phenomenon. In the following we demonstrate that the results obtained in refs.[3, 4] and [11] for spin tunneling between classically degenerate states in the presence of an applied magnetic field can essentially be obtained in a very simple way by comparison of the Schrödinger equation with that of a periodic potential for which the level splitting is well known, i.e. the Mathieu equation[16]. Apart from supplying a check of the path integral result, this type of derivation should appeal particularly to experimentalists. Moreover it has the enormous advantage of yielding automatically the extension to excited states which – as remarked earlier – is much more difficult to achieve with the path integral method. The calculation also gives a clearer picture of which parameters have to be large and which small for the results to have validity in the sense of asymptotic expansions.

In the following we concentrate on the case of a magnetic particle (e.g. an ion) embedded in the field of a crystal and a weak applied magnetic field $h = g\mu_B.\mathcal{B}$ perpendicular to the easy axis X. As explained in refs.[3, 4] for a specific model (among others) the appropriate Hamiltonian is

$$\hat{H} = -A\hat{S}_x^2 + B\hat{S}_z^2 - h\hat{S}_y \tag{1}$$

where A and B are positive anisotropy constants. One should note that two anisotropy axes are needed to produce tunneling when $h = 0$. After transforming the spin operators $\hat{S}_i$ to canonical operators $\hat{p}, \hat{\phi}$ [17] the relevant semiclassically approximated Hamiltonian can be written

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

where $[\hat{p}, \hat{\phi}] = i$ and

$$m(\phi) = \left[2(A\cos^2\phi + B) + \frac{h\sin\phi}{s+\frac{1}{2}}\right]^{-1} \tag{3}$$

and

$$V(\phi) = -\left[As(s+1)\cos^2\phi + h(s+\frac{1}{2})\sin\phi\right] \tag{4}$$

where s is the spin of the particle which is assumed to be not too small. The classical phase space is the unit sphere. The potential (which is two–fold degenerate for $h = 0$ in the domain $0 \leq \phi \leq \pi$ with easy axis X, i.e. the degenerate minima at 0 and π) can be seen to result from the Hamiltonian $\hat{H}$ obtained by replacing $\hat{S}_i$ by $s\mathbf{e}_i(\theta, \phi)$, $\mathbf{e}_i$ a unit vector expressed in polar coordinates, and replacing θ by its classical ground state value $\frac{\pi}{2}$. The derivation of the field dependence of the mass (which does not concern us here) is described in refs.[3, 4]. In the following we set

$$b = \frac{B}{A}, \quad a = \frac{h}{2A\left(s+\frac{1}{2}\right)} \tag{5}$$

and consider the experimentally interesting case of $b > 1$. Thus the mass $m(\phi)$ is to a first approximation given by $\frac{1}{2B}$. We demonstrated earlier[12] that corrections to this are small and can be taken into account in terms of elliptic functions (a modification which could, in principle, also be considered here but would overload this note with algebraic technicalities). We ignore these corrections in the first place.

The quantum states of the system (i.e. the degenerate states separated by infinitely high barriers) are determined by the oscillator approximation of the system around minimum positions ϕ_0 of V given by (with $s(s+1) \approx \left(s+\frac{1}{2}\right)^2$)

$$\sin\phi_0 = a, \quad \cos\phi_0 = \pm\sqrt{1-a^2} \tag{6}$$

and so

$$\phi_{0,2n} = 2n\pi + \arcsin a, \quad \phi_{0,2n+1} = (2n+1)\pi - \arcsin a, \quad n = 0, 1, 2, ... \tag{7}$$

with

$$\cos\phi_{0,2n} = +\sqrt{1-a^2}, \quad \cos\phi_{0,2n+1} = -\sqrt{1-a^2}$$

at which

$$V''(\phi_0) = 2As(s+1)[1-a^2] \equiv 8h_m^2.B \tag{8}$$

In the problem at hand $0 \leq \phi \leq 2\pi$ and there are only two minima as in the case of the well known double well potential. The Schrödinger equation $\hat{H}\Psi = E\Psi$ defined by $\hat{H}$ is then approximately

$$\Psi''(\phi) + \left[\frac{E - V(\phi_0)}{B} - 4h_m^2(\phi - \phi_0)^2\right]\Psi \simeq 0 \tag{9}$$

This determines immediately the oscillator approximated eigenvalues as

$$E_{2n+1}^{(0)} = -As(s+1) - \frac{h^2}{4A} + (2n+1)\sqrt{AB}\left(s + \frac{1}{2}\right)\sqrt{1-a^2} \tag{10}$$

in agreement with the "semiclassical ground state energy" ($n = 0$) given in ref.[3] (last formula) except that our B (assumed to be much larger than A) is there $B + A$. This perturbation theoretical expression ignores tunneling.

A typical aspect of any tunneling formula is the exponential of the euclidean action of the classical vacuum pseudoparticle (which tunnels through the barrier). This factor supplies the classical approximation of the transition amplitude equivalent to the wave function approximation given by the WKB exponential in quantum mechanics and must be such that it vanishes (i.e. the level splitting) in the limit of infinitely high barriers. In the present case this implies that h_m^2 has to be large and thus s or $As(s+1)$. The argument of the exponential must therefore contain s. In the path integral results of refs.[3, 4] the factors raised to powers of $2\left(s + \frac{1}{2}\right)$ play this role. In fact the factor in eq. (9a) of ref.[3] can be shown to approximate the WKB factor $exp(-\frac{2(s+\frac{1}{2})}{\sqrt{b}})$ in the limit of vanishing magnetic field h (one may note that $a = 1$ determines a critical value of h beyond which the degeneracy of minima for $h \neq 0$ – cf. eq.(6) – is removed as discussed by Schilling[11]). These observations suggest that the tunneling effect (i.e. the lifting of the degeneracy of oscillator levels) is calculable in much the same way as for periodic potentials, and that in fact the result can be obtained by identification of appropriate parameters. We do not enter into an extensive calculation here along the lines of ref.[16], and instead proceed by identification. One avoids ugly integrals by setting in the Schrödinger equation $E = E_{2n+1}^{(0)} + \triangle$, where $\triangle$ is the perturbation theory correction of the eigenvalue. The original Schrödinger equation then becomes

$$\Psi'' + \left\{-G^2(\phi) + (2n+1)\sqrt{\frac{A}{B}}\left(s + \frac{1}{2}\right)\sqrt{1-a^2} + \frac{\triangle}{B}\right\}\Psi = 0 \tag{11}$$

where

$$G^2(\phi) = \frac{\left(s+\frac{1}{2}\right)^2}{b}(\sin\phi - a)^2 \tag{12}$$

Setting

$$\Psi = \Xi(\phi)\exp\left\{\pm\int^{\phi} G(\phi)d\phi\right\}$$

we obtain the WKB exponential

$$\exp\left\{\pm\int^{\phi} G(\phi)d\phi\right\} = \exp\left\{\pm\frac{s+\frac{1}{2}}{\sqrt{b}}(\cos\phi + a\phi)\right\} \tag{13}$$

(note that without inclusion of the approximate form of E the integral would not have been so simple !). One can compute $\Xi(\phi)$ etc. as in ref.[16]. The boundary conditions require the evaluation of the wave function above the chosen minimum of the potential (say that at $\phi_{0,1}$), implying for the barriers to the left and to the right

$$\begin{aligned}
\int^{\phi_{0,1}} G(\phi)d\phi - \int^{\phi_{0,0}} G(\phi)d\phi &= \frac{2\left(s+\frac{1}{2}\right)}{\sqrt{b}}\left(\sqrt{1-a^2} + a\arcsin a - a\frac{\pi}{2}\right) \\
\int^{\phi_{0,1}} G(\phi)d\phi - \int^{\phi_{0.2}} G(\phi)d\phi &= \frac{2\left(s+\frac{1}{2}\right)}{\sqrt{b}}\left(\sqrt{1-a^2} + a\arcsin a + a\frac{\pi}{2}\right)
\end{aligned} \tag{14}$$

These expressions are seen to be (cf.ref.[10]) precisely the values of the action of the instantons travelling through the two differently sized barriers between $(\phi_{0,1}, \phi_{0,0})$ and $(\phi_{0,1}, \phi_{0,2})$ respectively as shown in Fig. 1 (one could say that these instantons describe clockwise and anticlockwise underbarrier rotations of the magnetic moment). In order to obtain this result it was essential to insert the oscillator approximated energy eq.(10) into the Schrödinger equation. It is exponential factors like those of eq.(13) with the boundary conditions of eq.(14) which are typical of tunneling contributions. In the present case both of these contribute to the overall level splitting. Knowing these factors we can write down the level splitting by making the appropriate replacements in the formula for the level splitting in the case of the Mathieu equation (cf. ref.[16] ,also cited in [12]) and adding these with equal weights so that in the limit $a \rightarrow 0$ we regain the level splitting of the case without the magnetic field. The factors multiplying the exponentials are characteristic of the central well (i.e. h_m^2 of eq.(8)) and in fact result from the matching of different branches of the wave function in domains of overlap as can be seen from ref.[16]; classically this factor describes the number of bounces of the particle between the barriers before it escapes. Thus these factors are the same in both cases so that from the level splitting result of ref.[16] (also cited in [12]) the level splitting of the nth excited state in the present case is obtained by the replacement

$$e^{-\frac{2\left(s+\frac{1}{2}\right)}{\sqrt{b}}} \rightarrow \frac{1}{2}e^{-\frac{2s}{\sqrt{b}}\left(\sqrt{1-a^2}+a\arcsin a\right)}.\left[e^{\frac{a\left(s+\frac{1}{2}\right)\pi}{\sqrt{b}}} + e^{-\frac{a\left(s+\frac{1}{2}\right)\pi}{\sqrt{b}}}\right]$$

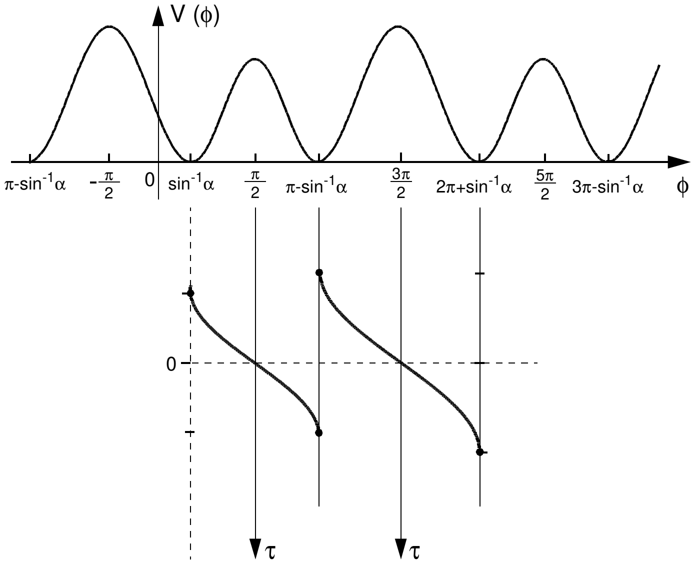

Figure 1: The periodic potential with asymmetric twin barriers and the instanton trajectories.

and hence is found to be

$$\triangle_{2n+1} = \frac{2B\left[\frac{8\left(s+\frac{1}{2}\right)}{\sqrt{b}}\sqrt{1-a^2}\right]^{n+\frac{3}{2}}}{\sqrt{8\pi}n!} \cdot e^{-\frac{2\left(s+\frac{1}{2}\right)}{\sqrt{b}}(\sqrt{1-a^2}+a\arcsin a)} \cdot \cosh\left(\frac{a\left(s+\frac{1}{2}\right)\pi}{\sqrt{b}}\right) \quad (15)$$

In the limit $a \to 0$ this reduces to the formula obtained in ref.[12] or to $\triangle E_0^{inst}$ of formula (9a) of ref.[3]. In particular we obtain for $n = 0$

$$\triangle_1 = \frac{16B}{\sqrt{\pi}}\left[\frac{s+\frac{1}{2}}{\sqrt{b}}\sqrt{1-a^2}\right]^{\frac{3}{2}} \cdot e^{-\frac{2\left(s+\frac{1}{2}\right)}{\sqrt{b}}(\sqrt{1-a^2}+a\arcsin a)} \cdot \cosh\left(\frac{a\left(s+\frac{1}{2}\right)\pi}{\sqrt{b}}\right) \quad (16)$$

which is to be compared with the corresponding path integral result of ref.[4] (there eq.(16)). In our result the origin of every factor is clearly understood as explained above - of course, with the assumption $B > A$ and $s > 1$. The somewhat different factors in ref.[4] result from the complicated path integral calculation, taking into account of the field dependence of the mass and appropriate approximations.

In Fig. 2 we plot our expression $\triangle_1$ for the values given in Fig. 2 of ref.[4]. We make the amazing observation that the plots are practically identical in spite of the fact that the value of b chosen (i.e. $b = 1$) is really too small and still better agreement with the exact values will be obtained for larger values of b.

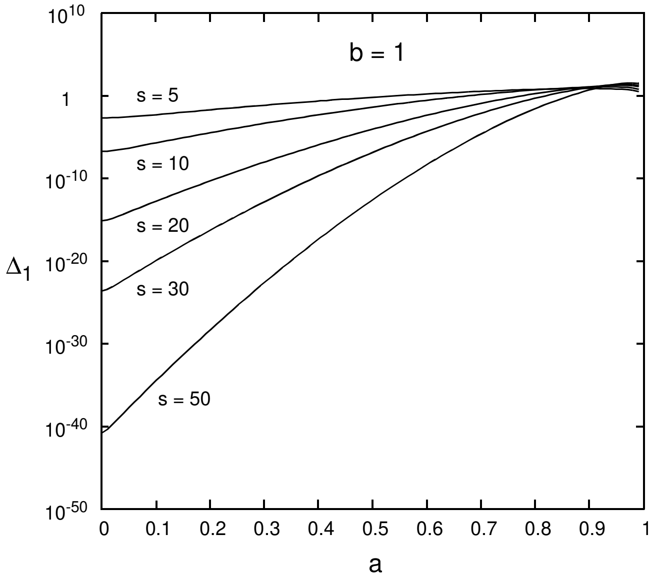

Figure 2: Logarithmic plot of $\triangle_1$ (in units of A) as a function of a for $b = \frac{B}{A} = 1$ and $s = 5, 10, 20, 30, 50$ to be compared with Fig. 2 of ref.[4].

In Figs.3 and 4 we display further plots of the level splitting demonstrating its increase with the magnetic field (as desired for better observability) and its variation with b for a fixed value of s.

In Table 1 we display some absolute values of the level splitting as calculated from our result and compare these with values given in ref.[3].

The very simple derivation of the nontrivial level splitting of eq.(16) given here demonstrates the calculational superiority of the Schrödinger method in quantum mechanics. Of course, the path integral method has considerable pedagogical value in quantum mechanics as a model for more complicated applications in field theory. The derivation given here also shows clearly that the parameters s and h_m^2 have to be large for the asymptotic expansions of the solutions and eigenvalues to make sense. One can also see that the effect of the field dependence of the mass – here neglected – cannot be large (in agreement with our findings in ref.[12]). A further considerable advantage of the derivation given here is – apart from checking the path integral result – that it immediately supplies the splitting of higher degenerate oscillator levels which cannot be obtained with vacuum instanton methods. It is interesting to observe that the WKB exponential which corresponds to the classical or tree approximation is the same also for excited states. Thus if this is calculated for nonvacuum (or periodic) instantons the same expression must be obtained. We did not specify above whether s is integral or half–integral. The reason is that for half

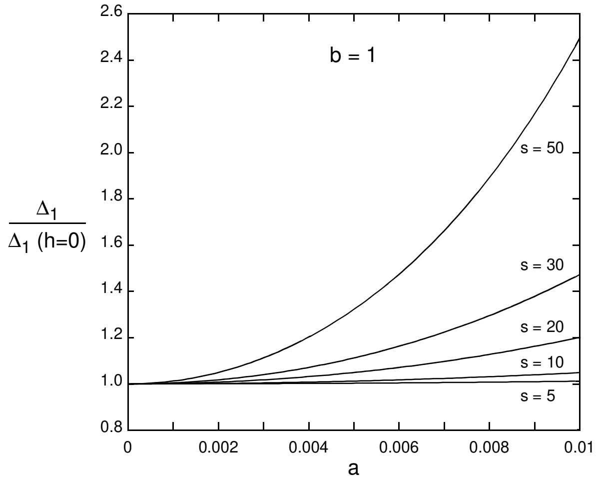

Figure 3: The ratio of the level splitting divided by that for $h = 0$ (i.e. magnetic field zero) plotted against a. One should note that a is effectively h divided by the large spin s.

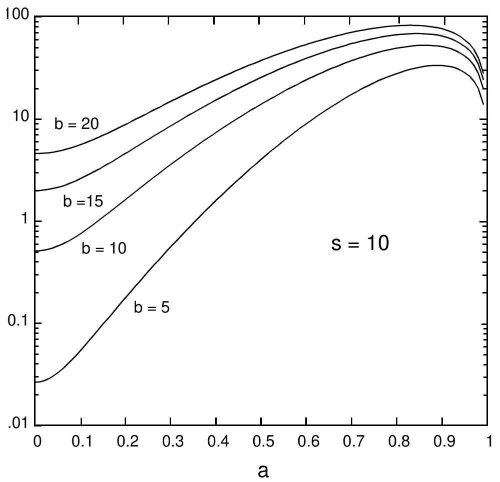

Figure 4: The level splitting at fixed value $s = 10$ for $b = 5, 10, 15$ and 20. In our considerations here b has to be larger than 1.

h	Δ_1	$\Delta_1/\Delta E_0$	$\Delta E_0^{inst}/\Delta E_0$
0.0	2.4488×10^{-4}	1.104	1.029
0.4	3.4375×10^{-4}	1.110	1.065
0.8	7.0830×10^{-4}	1.111	1.123
1.2	1.5803×10^{-3}	1.145	1.174

Table 1: Level splitting values calculated from Δ_1 in units of A compared with the numerical values ΔE_0 and the semiclassical results ΔE_0^{inst} of ref. [3] for $s = 10$, $b = 2$ and different values of h

integer spins the classical twofold degeneracy remains due to Kramer's degeneracy [8]. For completeness we mention that the case $B = 0$ has been dealt with in ref.[18], the method there employed being one applicable to the original discrete spin system. The method discussed here obviously also shows how the level splitting in the case of a periodic potential with periodically recurring asymmetric twin barriers can be obtained. We remark that numerous properties of spin systems have been considered in [19]. Finally our presentation should also appeal to experimentalists in view of the transparency of the calculational steps.

Acknowledgements

Two of us, J.–Q.L. (permanently at Department of Physics, Shanxi University, Taiyuan, P.R. China) and A.V.S. (permanently at Department of Mathematics, Georgian Academy of Sciences, Tbilisi, Georgia) are indebted to the Deutsche Forschungsgemeinschaft for financial support. The collaboration has also been supported by INTAS–93–1630 EXT.

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