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# Tunnelling of a large spin: mapping onto a particle problem

G Scharf†, W F Wreszinski† and J L van Hemmen‡

† Institut für Theoretische Physik der Universität Zürich, Schönberggasse 9, CH-8001 Zürich, Switzerland
‡ Sonderforschungsbereich 123 der Universität Heidelberg, D-6900 Heidelberg, Federal Republic of Germany

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**Abstract.** Tunnelling of a single quantum spin is studied in the limit of large spin quantum number $S$. The problem is mapped onto a *particle* problem on the positive half-line, with a Hamiltonian which is invariant under inversion $x \to 1/x$. Not only the ground-state energy but also all the other energy levels and corresponding level splittings (if any) are computed by using the conventional WKB methods for the particle problem and an excellent agreement with numerical data is found.

## 1. Introduction

In two recent papers (van Hemmen and Sütö 1986a, b) a WKB formalism was presented to describe the quantum dynamics, including tunnelling, of single spin with large spin quantum number $S$. A typical example is provided by the Schrödinger equation ($\hbar = 1$)

$$\mathrm{i}\frac{\mathrm{d}\psi}{\mathrm{d}t} = (-\gamma S_z^2 - \alpha S_x)\psi \tag{1.1}$$

of a spin with (large) anisotropy along the $z$ axis. Here $S_x$, $S_y$ and $S_z$ are dimensionless spin operators with commutators

$$[S_x, S_y] = \mathrm{i}S_z \tag{1.2}$$

and cyclic, and $\gamma > 0$. If $\hbar = 1$, the limit $S \to \infty$ makes no sense in (1.1) as it stands because the first term on the right is quadratic in $S$ whereas the second one is linear. The problem becomes well defined by multiplying (1.1) by $\gamma$,

$$\mathrm{i}\gamma\frac{\mathrm{d}\psi}{\mathrm{d}t} = (-\gamma^2 S_z^2 - \alpha\gamma S_x)\psi = H\psi \tag{1.3}$$

and considering the limit

$$S \to \infty \qquad \gamma \to 0 \qquad \gamma S = \text{constant}. \tag{1.4}$$

For the Hamiltonian (1.3), a tunnelling region appears when the anisotropy $-\gamma^2 S_z^2$ dominates the tunnelling term $-\alpha\gamma S_x$. In fact, as $\alpha \to 0$, the decay rate for the ground state $E_0 \approx -\gamma^2 S^2$ has been found to be given by (van Hemmen and Sütö 1986a, b)

$$\tau^{-1} = \frac{\gamma S}{\pi} \exp\left[-2S \log\left(\frac{\gamma S}{\alpha}\right)\right]. \tag{1.5}$$

In contrast to the particle case, we have a *logarithmic* dependence upon $\alpha$.

The simple formula (1.5) gives roughly the correct order of magnitude. In this paper we derive more accurate results for all pairwise nearly degenerate energy levels

$$E_M \approx -\gamma^2 M^2 \qquad M = \pm S, \pm(S-1)\ldots. \tag{1.6}$$

We obtain

$$\tau_M^{-1} = \frac{\Delta E_M}{\pi} = \frac{2}{\pi^2}\gamma M \exp J \tag{1.7}$$

with

$$J = -2M\left[\log\left(\frac{8}{\alpha}\gamma^2 M^2\right) - 1\right] + (2S+1)\log[\gamma(S+\tfrac{1}{2}+M)] - (S+\tfrac{1}{2}-M)\log\{\gamma^2[(S+\tfrac{1}{2})^2 - M^2]\} \qquad M > 0. \tag{1.8}$$

The formula (1.7) gives the correct level splittings $\Delta E_M$ up to an error on the per cent level for $S \geqslant 3$, $M \geqslant S/3$, say (see tables 1 and 2). In addition, we obtain the correction $O(\alpha^2)$ to the absolute energies (1.6)

$$E_M = -\gamma^2 M^2 - \frac{\alpha^2}{8}\left[\left(\frac{S+\frac{1}{2}}{M}\right)^2 + 1\right]. \tag{1.9}$$

The method we use was developed long ago (Scharf 1974, 1975) for another problem of large spin, namely the Dicke maser model. It runs as follows. There is an exact correspondence between the spin problem (1.3) and a quantum mechanical particle problem with one degree of freedom (§ 2). The limit $\gamma \to 0$ is just the semiclassical limit of this problem. The spectrum can therefore be calculated by the WKB method (§ 3).

A completely different approach to the level splitting, an instanton technique, has been advocated by Enz and Schilling (1986). See also Vourdas and Bishop (1985) and references quoted therein.

Hamiltonians of the form (1.3) are widely used to model anisotropies in spin glasses or other magnetic materials. At low temperatures, thermal activation is negligible and tunnelling remains as the only mechanism for the spins to relax to equilibrium.

## 2. Mapping onto a particle problem

The Hamiltonian (1.3) has the following two conserved quantities:

$$[H, S^2] = 0 \tag{2.1}$$

$$[H, C_2] = 0 \tag{2.2}$$

where

$$C_2 = \exp(\mathrm{i}\pi S_x) \tag{2.3}$$

is a rotation through $\pi$ about the $x$ axis. In the standard spin basis $|S, M\rangle$ we have

$$H|S, M\rangle = -\gamma^2 M^2 |S, M\rangle - \tfrac{1}{2}\alpha\gamma[(S+1+M)(S-M)]^{1/2}|S, M+1\rangle - \tfrac{1}{2}\alpha\gamma[(S+M)(S+1-M)]^{1/2}|S, M-1\rangle. \tag{2.4}$$

To get rid of the square root in (2.4) we transform the basis $|S, M\rangle$ as follows:

$$f_M = \binom{2S}{S+M}^{-1/2} |S, M\rangle \tag{2.5}$$

and get

$$Hf_M = -\gamma^2 M^2 f_M - \tfrac{1}{2}\alpha(S-M)f_{M+1} - \tfrac{1}{2}\alpha(S+M)f_{M-1}. \tag{2.6}$$

For the eigenvector

$$\psi = \sum_{M=-S}^{S} e_M f_M$$

we then obtain the eigenvalue equation

$$H\psi = -\gamma^2 \sum_M M^2 e_M f_M - \tfrac{1}{2}\alpha\gamma \sum_M (S-M) e_M f_{M+1} - \tfrac{1}{2}\alpha\gamma \sum_M (S+M) e_M f_{M-1} = E\psi. \tag{2.7}$$

The equation (2.7) is equivalent to

$$-\gamma^2 M^2 e_M - \tfrac{1}{2}\alpha\gamma(S-M+1)e_{M-1} - \tfrac{1}{2}\alpha\gamma(S+M+1)e_{M+1} = Ee_M \qquad M = -S, \ldots, +S \tag{2.8}$$

where

$$e_{-S-1} = 0 = e_{S+1}.$$

This automatically implies $e_{-S-2} = e_{S+2} = 0$, etc.

We now introduce the characteristic function

$$f(x) = \sum_{M=-S}^{S} e_M x^M. \tag{2.9}$$

Multiplying (2.8) by $x^M$ and summing over $M$, we get a second-order differential equation for $f$

$$-\gamma^2 x^2 f'' + (\tfrac{1}{2}\alpha\gamma x^2 - \gamma^2 x - \tfrac{1}{2}\alpha\gamma)f' - \tfrac{1}{2}\alpha\gamma S(x + x^{-1})f = Ef. \tag{2.10}$$

This equation can be transformed by a product ansatz into a Schrödinger form. There are various ways to do so. A unique transformation is selected by the requirement that the $C_2$ symmetry (2.2) is respected. This is very important for what follows. The $C_2$ transformation (2.3) means $M \to -M$, which corresponds to the inversion

$$x \to 1/x \tag{2.11}$$

in $f(x)$ defined by (2.9). With the product ansatz

$$y(x) = f(x) \exp\left(-\frac{\alpha}{4\gamma}(x + x^{-1})\right) \tag{2.12}$$

we obtain the *inversion-symmetric* equation

$$-\gamma^2(x^2 y'' + xy') + V(x)y \equiv \mathcal{H}y = Ey \tag{2.13}$$

with the potential

$$V(x) = \tfrac{1}{16}\alpha^2(x^2 + x^{-2} - 2) - \tfrac{1}{2}\alpha\gamma(S + \tfrac{1}{2})(x + x^{-1}). \tag{2.14}$$

The resulting Hamiltonian $\mathscr{H}$ is Hermitian on the Hilbert space $L^2_{1/x}(0,\infty)$ with scalar product

$$(\varphi,\psi)=\int_0^\infty \varphi(x)^*\psi(x)\,\mathrm{d}x/x. \tag{2.15}$$

It is possible to proceed to an ordinary $L^2$-space on the *whole* real line $(-\infty,\infty)$ by using the transformation

$$x=\mathrm{e}^z \tag{2.16}$$

of the independent variable. The resulting equation

$$-\gamma^2\frac{\mathrm{d}^2y}{\mathrm{d}z^2}+[\tfrac{1}{4}\alpha^2\sinh^2(z)-\alpha\gamma(S+\tfrac{1}{2})\cosh(z)]y(z)=Ey(z) \tag{2.17}$$

is invariant under reflection $z\to -z$. This formulation of the problem, however, is not convenient for the computations in the next section because the potential in (2.17) is transcendental instead of algebraic as in (2.14).

In the limit $S\to\infty$, $\gamma\to 0$, $\gamma S=\text{constant}$, the potential $V(x)$ in (2.14) becomes independent of $\gamma$,

$$V(x)=\tfrac{1}{16}\alpha^2(x+x^{-1})^2-\tfrac{1}{4}\alpha^2-\tfrac{1}{2}\alpha\sigma(x+x^{-1}) \tag{2.18}$$

with

$$\sigma=\gamma(S+\tfrac{1}{2}). \tag{2.19}$$

Furthermore, $\gamma$ enters in (2.13) and (2.17) in the same way as Planck's constant $\hbar$ in ordinary quantum mechanics. For this reason we can apply the WKB method (see, for example, Landau and Lifshitz (1965)). Maintaining the $\frac{1}{2}$ in (2.19), the results obtained are accurate even for small $S$, like $S=3$ (see table 1). The potential (2.18) is shown in figure 1. For $\sigma\gg\alpha$ there are two valleys, separated by a large barrier. This is the tunnelling region. For energies $E\sim-\sigma^2$, the tunnelling takes place between the two classical allowed regions

$$0<x_0<x_1<1 \qquad \text{and} \qquad 1<x_2<x_3 \tag{2.20}$$

**Table 1.** Ground-state energies $E_0$ and level splittings $\Delta E_0$ of the Hamiltonian $H=-S_z^2-S_x$ for $S=3,4,\ldots,11$; cf (1.7), (1.8) and (1.10).

| $S$ | $\lvert E_0\rvert$ numerical | $\lvert E_0\rvert$ analytical | $\Delta E_0$ numerical | $\Delta E_0$ analytical |
|---|---|---|---|---|
| 3 | 9.3015 | 9.2951 | $0.144\times10^{-2}$ | $0.150\times10^{-2}$ |
| 4 | 16.2860 | 16.2832 | $0.118\times10^{-4}$ | $0.118\times10^{-4}$ |
| 5 | 25.2779 | 25.2763 | $0.518\times10^{-7}$ | $0.511\times10^{-7}$ |
| 6 | 36.2728 | 36.2717 | $0.143\times10^{-9}$ | $0.139\times10^{-9}$ |
| 7 | 49.2693 | 49.2685 | $0.268\times10^{-12}$ | $0.259\times10^{-12}$ |
| 8 | 64.2667 | 64.2661 | $0.366\times10^{-15}$ | $0.352\times10^{-15}$ |
| 9 | 81.2647 | 81.2643 | $0.379\times10^{-18}$ | $0.363\times10^{-18}$ |
| 10 | 100.2632 | 100.2628 | $0.309\times10^{-21}$ | $0.295\times10^{-21}$ |
| 11 | 121.2619 | 121.2616 | $0.203\times10^{-24}$ | $0.193\times10^{-24}$ |

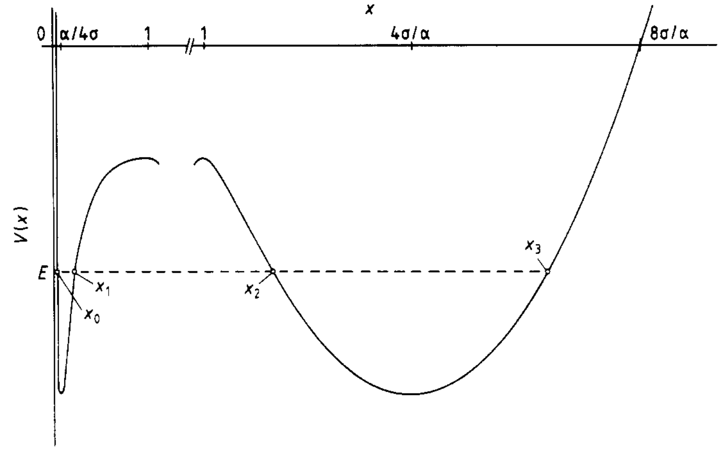


**Figure 1.** Double well potential $V(x)$ for $\alpha=1$, $\sigma=\gamma(S+\frac{1}{2})=3$. $x_0<x_1<1<x_2<x_3$ are the classical turning points for energy $E$. Two different scales have been chosen for $x\gtrless 1$, in order to make the two valleys visible.

where the classical turning points are given by

$$\begin{aligned} x_0 &= \frac{\alpha}{4|E|}(\sigma-Q) \\ x_1 &= \frac{\alpha}{4|E|}(\sigma+Q) \ll 1 \\ x_2 &= \frac{4}{\alpha}(\sigma-Q)=\frac{1}{x_1} \\ x_3 &= \frac{4}{\alpha}(\sigma+Q)=\frac{1}{x_0} \end{aligned} \tag{2.21}$$

with

$$Q=(\sigma^2-|E|)^{1/2} \tag{2.22}$$

$$\alpha \ll |E|^{1/2}\sim\sigma. \tag{2.23}$$

## 3. WKB treatment

Introducing the WKB ansatz

$$y(x)=\exp\left(\frac{\mathrm{i}}{\gamma}S(x)\right) \tag{3.1}$$

into (2.13) we obtain

$$x^2S'^2-\mathrm{i}\gamma x^2S''-\mathrm{i}\gamma xS'=E-V. \tag{3.2}$$

We expand

$$S=S_0+\frac{\gamma}{\mathrm{i}}S_1+\mathrm{O}(\gamma^2) \tag{3.3}$$

and arrive in lowest order O(1) at the classical Hamilton-Jacobi equation

$$x^2 S_0'^2 = E - V \tag{3.4}$$

with the solution

$$S_0(x) = \int^x (E - V(x'))^{1/2} \frac{\mathrm{d}x'}{x'}. \tag{3.5}$$

The equation of order $\gamma$ for $S_1$,

$$S_1' = -\frac{S_0''}{2S_0'} - \frac{1}{2x} \tag{3.6}$$

gives

$$S_1(x) = -\tfrac{1}{4}\log|E - V(x)| + \text{constant}. \tag{3.7}$$

By the standard connection argument, we obtain the wavefunction in the classically allowed region $x_0 < x < x_1$

$$y(x) = C(E - V)^{-1/4} \cos\left(\frac{1}{\gamma}\int_{x_1}^x (E - V)^{1/2} \frac{\mathrm{d}x'}{x'} + \frac{\pi}{4}\right). \tag{3.8}$$

The Bohr-Sommerfeld eigenvalues $E_n$ are determined by the transcendental equation

$$\frac{1}{\gamma}\int_x^{x_1} (E_n - V(x))^{1/2} \frac{\mathrm{d}x}{x} = \pi(n + \tfrac{1}{2}) \qquad n = 0, 1, \ldots . \tag{3.9}$$

The resulting elliptic integral

$$\int_{x_0}^{x_1} [-\tfrac{1}{16}\alpha^2 x'^4 + \tfrac{1}{2}\alpha\sigma x'^3 + (E_n + \tfrac{1}{8}\alpha^2)x'^2 + \tfrac{1}{2}\alpha\sigma x' - \tfrac{1}{16}\alpha^2]^{1/2} \frac{\mathrm{d}x'}{x'^2} \tag{3.10}$$

need not be computed as it stands, because we have by (2.21)

$$x' \approx \frac{\alpha\sigma}{4|E_n|} = \mathrm{O}\left(\frac{\alpha}{\sigma}\right) \tag{3.11}$$

on the average. The leading-order integral is elementary

$$\int_{x_0}^{x_1} (E_n x'^2 + \tfrac{1}{2}\alpha\sigma x' - \tfrac{1}{16}\alpha^2)^{1/2} \frac{\mathrm{d}x'}{x'^2} = [\sigma - |E_n|^{1/2}]\pi. \tag{3.12}$$

It follows from (3.9) that

$$|E_n|^{1/2} = \sigma - (n + \tfrac{1}{2})\gamma = (S - n)\gamma. \tag{3.13}$$

Putting

$$S - n = M \tag{3.14a}$$

we get the unperturbed spin eigenvalues

$$|E_M| = \gamma^2 M^2. \tag{3.14b}$$

The corrections to them are of order $\alpha^2$ and come from the cubic $(\frac{1}{2}\alpha\sigma x'^3)$ and quadratic $(\frac{1}{8}\alpha^2 x'^2)$ terms in (3.10). For the lower part of the spectrum we may approximate $x'$ by its mean value (3.11) in

$$\tfrac{1}{2}\alpha\sigma x'^3 \approx \tfrac{1}{2}\alpha\sigma\frac{\alpha\sigma}{4|E_n|}x'^2 \approx \frac{\alpha^2\sigma^2}{8\gamma^2 M^2}x'^2.$$

The resulting modification

$$E_n = -|E_n| \to -|E_n| + \tfrac{1}{8}\alpha^2\left(1+\frac{\sigma^2}{\gamma^2 M^2}\right)$$

leads to the corrected eigenvalues

$$|E_M| = \gamma^2 M^2 + \tfrac{1}{8}\alpha^2\left[1+\left(\frac{S+\frac{1}{2}}{M}\right)^2\right]. \tag{3.15}$$

As can be seen from tables 1 and 2 there is good agreement with numerical results except for the highest energies.

**Table 2.** Energy levels $E_M$ and level splittings $\Delta E_M$ of the Hamiltonian $H = -S_z^2 - S_x$ for $S = 10$, $M = 10, 9, \ldots, 3$; cf (1.7), (1.8) and (1.10).

| $M$ | $\lvert E_M\rvert$ numerical | $\lvert E_M\rvert$ analytical | $\Delta E_M$ numerical | $\Delta E_M$ analytical |
|---|---|---|---|---|
| 10 | 100.2632 | 100.2628 | $0.309\times10^{-21}$ | $0.295\times10^{-21}$ |
| 9 | 81.2957 | 81.2951 | $0.718\times10^{-17}$ | $0.722\times10^{-17}$ |
| 8 | 64.3414 | 64.3403 | $0.554\times10^{-13}$ | $0.569\times10^{-13}$ |
| 7 | 49.4082 | 49.4063 | $0.178\times10^{-9}$ | $0.187\times10^{-9}$ |
| 6 | 36.5122 | 36.5078 | $0.248\times10^{-6}$ | $0.269\times10^{-6}$ |
| 5 | 25.6884 | 25.6763 | $0.141\times10^{-3}$ | $0.164\times10^{-3}$ |
| 4 | 17.02 | 16.99 | $0.276\times10^{-1}$ | $0.379\times10^{-1}$ |
| 3 | 10.04 | 10.66 | 0.974 | 2.75 |

Now we turn to tunnelling. We adapt a method of Landau and Lifshitz (1965) to the inversion-symmetric Hamiltonian (2.13)

$$-\gamma^2(x^2\psi'' + x\psi') + V(x)\psi = E\psi. \tag{3.16}$$

The eigenfunctions of the two nearly degenerate states in the double well can be expressed as

$$\psi_1(x) = 2^{-1/2}[\psi_0(x) + \psi_0(x^{-1})] \tag{3.17}$$

$$\psi_2(x) = 2^{-1/2}[\psi_0(x) - \psi_0(x^{-1})] \tag{3.18}$$

where $\psi_0(x)$ is a real eigenfunction for a single well in the interval [0, 1], say,

$$-\gamma^2(x^2\psi_0'' + x\psi_0') + V(x)\psi_0 = E_0\psi_0 \qquad 0 < x \leqslant 1. \tag{3.19}$$

We normalise $\psi_0$ according to

$$\int_0^1 \psi_0^2(x)\frac{\mathrm{d}x}{x} = 1. \tag{3.20}$$

Multiplying the eigenvalue equation for $\psi_1$

$$-\gamma^2(x^2\psi_1'' + x\psi_1') + V(x)\psi_1 = E_1\psi_1$$

by $\psi_0$ and (3.19) by $\psi_1$, subtracting and integrating from 0 to 1, we get

$$-\gamma^2 \int_0^1 \mathrm{d}x\, x \frac{\mathrm{d}}{\mathrm{d}x} (\psi_1' \psi_0 - \psi_1 \psi_0') - \gamma^2 \int_0^1 \mathrm{d}x (\psi_1' \psi_0 - \psi_0 \psi_1')$$
$$= (E_1 - E_0) \int_0^1 \frac{\mathrm{d}x}{x} \psi_1 \psi_0$$
$$= (E_1 - E_0) \int_0^1 \frac{\mathrm{d}x}{x} \frac{\psi_0}{\sqrt{2}} \psi_0 = 2^{-1/2} (E_1 - E_0) \tag{3.21}$$

because $\psi_0(x^{-1})$ in (3.17) is exponentially small in the interval $0 < x \leqslant 1$. Simplifying the left-hand side of (3.21) by partial integration, we arrive at

$$2^{-1/2}(E_1 - E_0) = -\gamma^2 [x(\psi_0 \psi_1' - \psi_1 \psi_0')](1)$$
$$= 2^{1/2} \gamma^2 \psi_0(1) \psi_0'(1) \tag{3.22}$$

or simply

$$E_1 - E_0 = 2\gamma^2 \psi_0(1) \psi_0'(1).$$

Proceeding in the same way with $\psi_2$ of (3.18), we obtain

$$E_2 - E_0 = -2\gamma^2 \psi_0(1) \psi_0'(1)$$

which leads to the splitting of the eigenvalues

$$\Delta E = E_2 - E_1 = -4\gamma^2 \psi_0(1) \psi_0'(1). \tag{3.23}$$

Here we need the WKB wavefunction in the forbidden region $x_1 < x \leqslant 1$

$$\psi_0(x) = \tfrac{1}{2} c (V - E)^{-1/4} \exp\left( -\frac{1}{\gamma} \int_{x_1}^{x} (V - E)^{1/2} \frac{\mathrm{d}x'}{x'} \right). \tag{3.24}$$

The normalisation constant is determined by matching to (3.8). In the normalisation integral the contribution of the forbidden region can be neglected compared with the contribution of the allowed region (3.8). For small $\gamma$, $\cos^2(\ldots)$ may on the average be approximated by $\frac{1}{2}$, so that

$$1 = \tfrac{1}{2} c^2 \int_{x_0}^{x_1} \frac{\mathrm{d}x}{x(E - V(x))^{1/2}}.$$

Here we can again use the quadratic approximation under the square root which gives

$$c^2 = \frac{2}{\pi} |E|^{1/2}. \tag{3.25}$$

For the derivative in (3.23), we have to leading order in $\gamma$, only to differentiate the exponent in (3.24). This leads to

$$\Delta E = \frac{2}{\pi} \gamma |E|^{1/2} \exp J \tag{3.26}$$

with

$$J = -\frac{2}{\gamma} \int_{x_1}^{1} (V - E)^{1/2} \frac{\mathrm{d}x}{x} = -\frac{1}{\gamma} \int_{x_1}^{x_2} (V(x) - E)^{1/2} \frac{\mathrm{d}x}{x}. \tag{3.27}$$

Here we cannot avoid computing the elliptic integral. This is done in the appendix. The result is

$$J = -\frac{2}{\gamma} \left\{ |E|^{1/2} \left[ \log\left( \frac{8}{\alpha} |E| \right) - 1 \right] - \sigma \log(\sigma + |E|^{1/2}) + (\sigma - |E|^{1/2}) \log(\sigma^2 - |E|)^{1/2} \right\}. \tag{3.28}$$

Substituting

$$|E_M| = \gamma^2 M^2 \qquad \sigma = \gamma(S+\tfrac{1}{2})$$

we have the following final result for the level splitting (3.26):

$$\Delta E_M = \frac{2}{\pi}\,\gamma M \exp J \qquad M>0 \tag{3.29}$$

with

$$J = -2M\left[\log\left(\frac{8}{\alpha}\,\gamma^2 M^2\right) - 1\right] + (2S+1)\log[\gamma(S+\tfrac{1}{2}+M)] \\ -(S+\tfrac{1}{2}-M)\log\{\gamma^2[(S+\tfrac{1}{2})^2 - M^2]\} \tag{3.30}$$

as announced in § 1.

We have compared the predictions of (3.29) and (3.30) with numerical calculations for $S = 3, 4, \ldots, 11$. Even for $\alpha = 1$ the agreement is remarkably good (tables 1 and 2), despite the fact that there is a rapid exponential variation of $\Delta E_M$ with $M$. Only the highest eigenvalues $|M| < S/3$, say, are inaccurate, because there is no longer any tunnelling barrier.

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## Appendix

We decompose $J$ in (3.27) as follows:

$$J = -\frac{2}{\gamma}(J_1 + J_2 + J_3 + J_4 + J_5) \tag{A1}$$

$$J_1 = -(E + \tfrac{1}{8}\alpha^2)\int_{x_1}^{x_2} \frac{\mathrm{d}x}{(R(x))^{1/2}} \tag{A2}$$

$$J_2 = -\tfrac{1}{2}\alpha\sigma \int_{x_1}^{x_2} \frac{\mathrm{d}x}{x(R(x))^{1/2}} \tag{A3}$$

$$J_3 = \tfrac{1}{16}\alpha^2 \int_{x_1}^{x_2} \frac{\mathrm{d}x}{x^2(R(x))^{1/2}} \tag{A4}$$

$$J_4 = -\tfrac{1}{2}\alpha\sigma \int_{x_1}^{x_2} \frac{x\,\mathrm{d}x}{(R(x))^{1/2}} \tag{A5}$$

$$J_5 = \tfrac{1}{16}\alpha^2 \int_{x_1}^{x_2} \frac{x^2\,\mathrm{d}x}{(R(x))^{1/2}} \tag{A6}$$

with

$$R(x)=\tfrac{1}{16}\alpha^2x^4-\tfrac{1}{2}\alpha\sigma x^3-(E+\tfrac{1}{8}\alpha^2)x^2-\tfrac{1}{2}\alpha\sigma x+\tfrac{1}{16}\alpha^2$$
$$=(\tfrac{1}{4}\alpha)^2(x_3-x)(x_2-x)(x-x_1)(x-x_0). \tag{A7}$$

We have

$$J_2=J_4 \qquad J_3=J_5$$

by inversion symmetry. $J_1$ is an elliptic integral of the first kind

$$J_1=|E|^{1/2}K(k'^2) \tag{A8}$$

where

$$k'^2=1-k^2$$
$$k^2=\frac{\alpha^2}{4}\frac{\sigma^2-|E|}{E^2}\ll 1. \tag{A9}$$

The integrals $J_2$ and $J_3$ can be expressed by complete elliptic integrals of the first $K(k'^2)$, second $E(k'^2)$ and third kind $\Pi(\beta^2, k'^2)$ (Byrd and Friedman 1971):

$$J_2=-\sigma g[x_3K(k'^2)+(x_2-x_3)\Pi(\beta^2,k'^2)] \tag{A10}$$

$$J_3=\tfrac{1}{8}\alpha x_2^2\frac{g}{\beta^4}\Bigg(\beta_1^4K+2\beta_1^2(\beta^2-\beta_1^2)\Pi$$
$$+\frac{(\beta^2-\beta_1^2)^2}{2(\beta^2-1)(k'^2-\beta^2)}[\beta^2E(k'^2)+(k'^2-\beta^2)K$$
$$+(2\beta^2k'^2+2\beta^2-\beta^4-3k'^2)\Pi]\Bigg) \tag{A11}$$

with

$$g=\frac{2}{[(x_3-x_1)(x^2-x_0)]^{1/2}}\approx\frac{\alpha}{2|E|^{1/2}}$$
$$\beta^2=\frac{x_2-x_1}{x_3-x_1}\approx\frac{[\sigma-(\sigma^2-|E|)^{1/2}]^2}{|E|} \tag{A12}$$
$$\beta_1^2=\frac{x_3}{x_2}\beta^2=1-\frac{\alpha^2}{8E^2}[\sigma^2-|E|+\sigma(\sigma^2-|E|)^{1/2}].$$

$\Pi$ can be computed in terms of incomplete integrals of the first $F$ and second kind $E$ (Byrd and Friedman 1971):

$$\Pi(\beta^2,k'^2)=K(k'^2)+\frac{\beta}{[(1-\beta^2)(k'^2-\beta^2)]^{1/2}}$$
$$\times(K(k'^2)E(\delta,k')-E(k'^2)F(\delta,k')) \tag{A13}$$

with

$$\sin\delta=\frac{\beta}{k'}=\beta\left[1+O\left(\frac{\alpha^2}{|E|}\right)\right].$$

For $k'$ near 1, the following approximate expressions are valid (Byrd and Friedman 1971):

$$K(k'^2) = \log \frac{4}{k}$$

$$E(k'^2) = 1$$

$$F(\delta, k') = \log \frac{1 + \sin \delta}{\cos \delta}$$

$$E(\delta, k') = \sin \delta.$$

Putting everything together we obtain

$$J_1 + 2J_2 + 2J_3 = |E|^{1/2}\{\log[(8/\alpha)|E|] - 1\} - \sigma \log(\sigma + |E|^{1/2}) + (\sigma - |E|^{1/2}) \log(\sigma^2 - |E|)^{1/2}. \tag{A14}$$

This result is used in (3.28) in the main text.

## References


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