RESULTS for SPIN TUNNELING

Considering how hard the solution of the problem of a spin-½ is in general, it will come as no surprise that the general dynamics of a higher spin is extremely complex. However one problem, of quite exceptional interest in the last 2 decades, is actually amenable to fairly accurate treatment. This is the spin analogue of tunneling, in which the spin rotates from one orientation to another through a classically forbidden region. The results are of general methodological interest, since they allow for treatment using both non-perturbative (WKB) and perturbative methods; and the problem is amenable to a very elegant treatment using path integrals. Some interesting subtleties of coherent states become evident in this treatment.

This problem is of particular interest because in the last decade it has become experimentally accessible. This has allowed direct verification of some of the more spectacular "spin phase" effects.

1. SIMPLE EXAMPLES

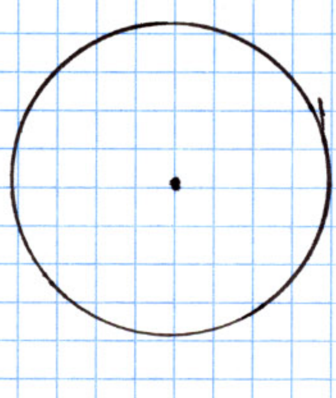
We are in general interested in a spin $\underline{S}$ (in experiments, $S = |\underline{S}|/\hbar$ can range from ½ to ~ 30), which is governed by a Hamiltonian $\mathcal{H}_0(\hat{\underline{S}})$ which can be written as a polynomial in $\hat{S}_x, \hat{S}_y, \hat{S}_z$, of maximum degree $2S$. Clearly for large S, we are dealing with a huge range of possible forms for $\mathcal{H}_0(\underline{S})$.

To focus the discussion we consider 3 examples.

1.(a) BIAXIAL TUNNELING SPIN IN A FIELD

: This is the simplest example, to which most attention has been given in the literature. We have a Hamiltonian which we will choose, to be specific, of easy axis form:

$$\left.\begin{aligned}\mathcal{H}_0(\underline{S}) &= -K_z \hat{S}_z^2 + K_\perp(\hat{S}_x^2 - \hat{S}_y^2) \\ &\equiv \frac{\hbar}{S}\left[-\bar{K}_z \hat{S}_z^2 + \bar{K}_\perp(\hat{S}_x^2 - \hat{S}_y^2)\right]\end{aligned}\right\} \quad (1)$$

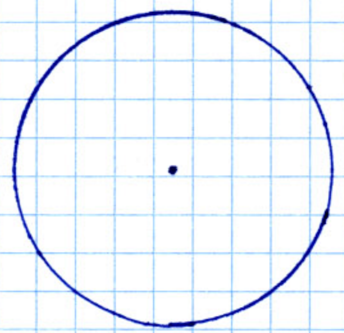


where the 2nd form shows explicitly that the Hamiltonian is $\sim O(S)$; this is the case for all terms in it. We also write this as

$$\mathcal{H}_0(\underline{S}) = \frac{\hbar}{S}\left[-\bar{K}_z \hat{S}_z^2 + \tfrac{1}{2}\bar{K}_\perp(\hat{S}_+^2 + \hat{S}_-^2)\right] \quad (2)$$

where as usual, $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. Now we notice here that there are no higher terms in the $\hat{S}_\alpha$; this is an approximation if $S > 1$, because such terms are permitted. However

We also notice that the Hamiltonian only contains terms even in the spin components - this reflects the assumption that the system is inversion-symmetric. The easiest way to get a term which is odd in $\underline{S}$ is to add a magnetic field, which here gives a Hamiltonian



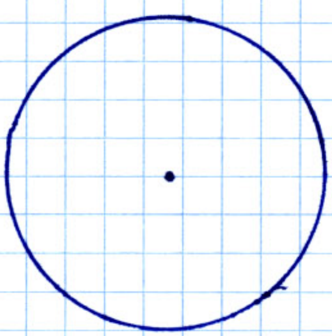
$$\mathcal{H}(\underline{S}) = \mathcal{H}_0(\underline{S}) - \gamma_{\alpha\beta} S^\alpha H_0^\beta \quad (3)$$

where

$$\gamma_{\alpha\beta} = \mu_B g_{\alpha\beta} \quad (4)$$

(a) FIELD ALONG $\hat{\underline{x}}$

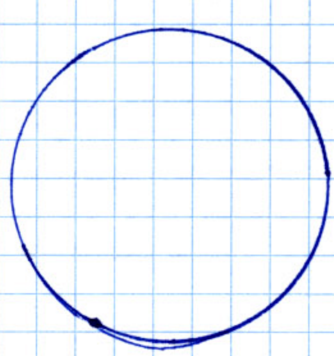
A magnetic field has a profound influence on the tunneling dynamics of a spin, as we might expect. We see this intuitively at left; two situations are shown, both involving a field transverse to the easy axis.



In the case shown above (in (a)), we have the field along the hard axis (the one with highest energy), the effect is to lower the energy of the paths between the 2 minima, which themselves move away from the poles towards each other. Note the problem is still reflection-symmetric, about the xz-plane. In the case (b) shown below, the field is along $\hat{\underline{y}}$, and one sees a range of intermediate cases with $\underline{H}_0$ oriented in the xy-plane, somewhere between $\hat{\underline{x}}$ and $\hat{\underline{y}}$.

(b) FIELD ALONG $\hat{\underline{y}}$

The contour lines of equipotential for the equivalent classical potential are shown in these figures. This classical potential assumes that $\hat{S}$, the operator is substituted by $\hbar S \underline{n}$, the continuous potential on the Bloch sphere. This then gives the potential



$$\mathcal{H}_0(\hbar S \underline{n}) = \hbar S \left[\bar{K}_\parallel \sin^2\theta + \bar{K}_\perp \sin^2\theta \cos 2\phi \right] \quad (5)$$

with (θ, ϕ) the Bloch sphere angles. Notice that if $\bar{K}_\perp = 0$, we have the very simple easy axis potential shown at left. It will be obvious from the form of the Hamiltonian in this case that no transitions are possible between eigenstates of $|\hat{S}_z\rangle$, since this is now conserved. This should be a caution against any naive idea that the system moves along paths perpendicular to the equipotentials – in this case there would be nothing to stop any tunneling between the north and south poles in this pure easy axis potential. We look at this properly in the context of a path integral formulation of the problem, later on.

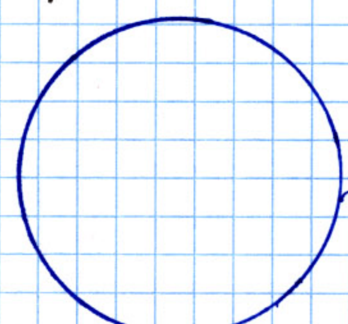
Finally, note that we can write the Hamiltonian in terms of what are known as "Stevens operators" (for details see appendix), in the form

$$\left.\begin{aligned} \mathcal{H}_o(\underline{S}) &= -\frac{K_z}{3}\hat{O}_2^0 + K_\perp \hat{O}_2^2 \\ &= \frac{\hbar}{S}\left[-k_z/3\, \hat{O}_2^0 + \bar{k}_\perp \hat{O}_2^2\right] \end{aligned}\right\} \quad (6)$$

There are many examples in solid-state physics of systems described very well by a Hamiltonian of this kind. One of these which has been investigated most thoroughly is the "Fe_8 molecule"; however it also has an important 4th-order term. It's Hamiltonian is

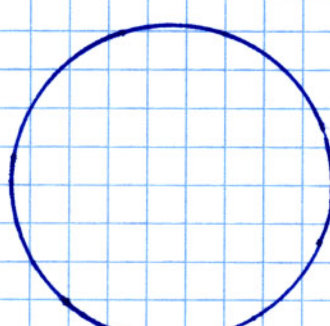
$$\left.\begin{aligned} \mathcal{H}_o(\underline{S}) &= D_o\hat{S}_z^2 + E_o\hat{S}_x^2 + \tfrac{1}{2}K_4^\perp(S_+^4 + S_-^4) + K_4^z S_z^4 \\ &= K_2^z\hat{S}_z^2 + \tfrac{1}{2}K_2^\perp(\hat{S}_+^2 + \hat{S}_-^2) + \tfrac{1}{2}K_4^\perp(\hat{S}_+^4 + \hat{S}_-^4) + K_4^z S_z^4 \end{aligned}\right\} \quad (7)$$

where in the first form we use another familiar notation. For the Fe_8 system, there is also a rather small term which mixes together S_z and $S_\pm$ operators, of form $\sim \hat{S}_z^2(\hat{S}_+^2 + \hat{S}_-^2)$, which we ignore here. The values of these parameters that we will use for Fe_8 are:



$$\left.\begin{aligned} D_o &= -0.23\,K \\ E_o &= 0.094\,K \\ K_4^\perp &= -6.56\times 10^{-5}\,K \end{aligned}\right\} \quad (8)$$

which correspond to



$$\left.\begin{aligned} K_2^z &= -0.277\,K \\ K_2^\perp &= 0.047\,K \end{aligned}\right\} \quad (9)$$

since

$$\left.\begin{aligned} K_2^z &= D_o - E_o/2 \\ K_2^\perp &= E_o/2 \end{aligned}\right\} \quad (10)$$

Here we neglect the term K_4^z, which is actually very small. The forms in (7), along with the numbers in (8) & (9), are very misleading in one as we see if we rewrite $\mathcal{H}_0(\underline{S})$ as

$$\left.\begin{aligned} \mathcal{H}_0(S) &= \hbar S\left\{\left[\bar{k}_2^z \cos^2\theta + \bar{k}_2^\perp \sin^2\theta\cos 2\phi\right] + \left[\bar{k}_4^z \cos^4\theta + \bar{k}_4^\perp \sin^4\theta \cos 4\phi\right]\right\} \\ &\equiv \hbar\left\{\frac{1}{S}\left[\bar{k}_2^z \hat{S}_z^2 + \tfrac{1}{2}\bar{k}_2^\perp(\hat{S}_+^2 + \hat{S}_-^2)\right] + \frac{1}{S^3}\left[k_4^z \hat{S}_z^4 + \tfrac{1}{2}k_4^\perp(\hat{S}_+^4 + \hat{S}_-^4)\right]\right\} \end{aligned}\right\} \quad (11)$$

in which case the parameters are

$$\left.\begin{aligned} \hbar\bar{k}_2^z &= -2.77\,K & \hbar\bar{k}_2^\perp &= 0.47\,K \\ \hbar\bar{k}_4^z &= 0 & \hbar\bar{k}_4^\perp &= -6.56\times10^{-2}\,K \end{aligned}\right\} \quad (12)$$

We see that in reality the 4th-order parameter $\bar{k}_4$ is only ~ 7 times smaller than $\bar{k}_2^\perp$, rather than 700 times smaller as one might infer from (8) and (9). We shall see later on that the effects of $\bar{k}_4^\perp$ are rather profound.

These results indicate that a study of the general biaxial system with quartic terms may be rather interesting. The most general form may be written, assuming inversion symmetry, as

$$\left.\begin{aligned} \mathcal{H}_0(S) &= \sum_{2l=-2}^{2} B_2^{2l}\hat{O}_2^{2l} + \sum_{2l=-4}^{4} B_4^{2l}\hat{O}_4^{2l} \\ &\equiv \left[K_2^z \hat{S}_z^2 + K_2^x \hat{S}_x^2 + K_2^y \hat{S}_y^2 \right. \\ &\qquad \left. + K_4^{zz} S_z^4 + K_4^{zx} S_z^2 S_x^2 + K_4^{zy} S_z^2 S_y^2 + K_4^{xy} S_x^2 S_y^2\right] \end{aligned}\right\} \quad (13)$$

This form is too complicated for a general analysis here.

1.(b) <u>COMBINED QUARTIC/SEXTIC HAMILTONIAN</u>

: As one increases the complexity of terms in $\mathcal{H}_0(S)$ by increasing the order in S_α of the terms. It is thus not immediately obvious what is gained by analyzing a 6th-order Hamiltonian. However it turns out to be quite interesting to look at a system in which the effects of 4th-order and 6th-order terms compete; in the same way as for the competition between 2nd-order & 4th-order terms noted above, the results can be rather surprising.

The most general form for a 6th-order Hamiltonian is

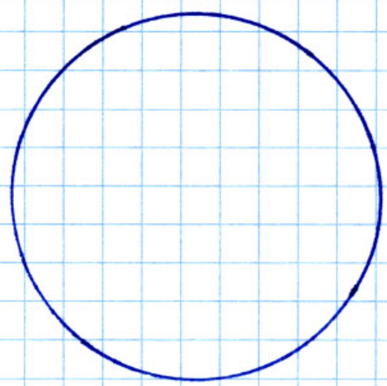
$$\left.\begin{aligned} \mathcal{H}_0(\underline{S}) &= \sum_{2m=1}^{3}\sum_{2l=-2m}^{2m} B_{2m}^{2l}\hat{O}_{2m}^{2l} \\ &= \sum_{2l=-2}^{2} B_2^{2l}\hat{O}_2^{2l} + \sum_{2l=-4}^{4} B_4^{2l}\hat{O}_4^{2l} + \sum_{2l=-6}^{6} B_6^{2l}\hat{O}_6^{2l} \end{aligned}\right\} \quad (14)$$

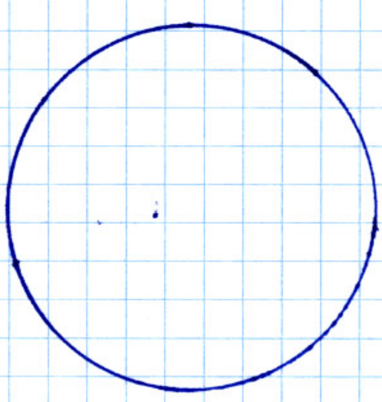
but we shall only be interested in the following special case of this Hamiltonian, viz.,

$$\mathcal{H}_0(\underline{S}) = \hbar\left\{ \frac{\bar{k}_2^z}{S}\hat{S}_z^2 + \frac{1}{S^3}\left[\bar{k}_4^z \hat{S}_z^4 + \tfrac{1}{2}\bar{k}_4^4(\hat{S}_+^4+\hat{S}_-^4)\right] + \frac{1}{S^5}\left[\bar{k}_6^z\hat{S}_z^6 + \tfrac{1}{2}\bar{k}_6^4(\hat{S}_+^4+\hat{S}_-^4)\hat{S}_z^2\right]\right\} \qquad (15)$$

In this Hamiltonian we exclude terms in $(S_+^6 \pm S_-^6)$, which would introduce a 6-fold symmetry in the potential w.r.t. rotations about the $\hat{z}$-axis. Notice that only changes Δm in $S_z/\hbar$ satisfying $\Delta m = \pm 4$ are allowed by this Hamiltonian. The equivalent classical Hamiltonian is

$$\mathcal{H}_0(\underline{S}) = \hbar S\left\{\bar{k}_2^z\cos^2\theta + \left[k_4^z\cos^4\theta + \bar{k}_4^4\sin^4\theta\cos 4\phi\right] + \left[\bar{k}_6^z\cos^6\theta + \bar{k}_6^4\cos^2\theta\sin^4\theta\cos 4\phi\right]\right\} \qquad (16)$$





Again, the form that the classical potential takes on the Bloch sphere depends very much on the sign & magnitude of the coefficients in (16). At left we plot one possible version, chosen to illustrate some of the basic features. As the multiplicity in S of the polynomial terms in $\mathcal{H}_0(\underline{S})$ increases, the system of potential wells becomes very intricate - moreover, its sensitivity to small changes in the coefficients of these parameters also becomes important. This means that one can manipulate the spin dynamics using applied fields, producing a variety of different behaviours.

As we will discuss later, there is a very nice example of this kind of system that has been very heavily studied in experiments - this is the $LiHo_xY_{1-x}F_4$ system. The effective Hamiltonian for each Ho ion, for which $S = 8$, has the parameters

$$\begin{aligned} B_2^0 &= -0.696\ K \qquad & B_4^0 &= 4.06\times10^{-3}\ K \qquad & B_6^0 &= 4.64\times10^{-6}\ K \\ & & B_4^4 &= 4.18\times10^{-2}\ K \qquad & B_6^4 &= 8.12\times10^{-4}\ K \end{aligned} \qquad (17)$$

with all others negligible.

1. (c) TUNNELING SPIN DIMERS:

An obvious question to ask about the dynamics of spin systems, particularly when they are tunneling, is - how do a pair of coupled spins affect each others' tunneling, and what new features emerge? To address this question, we consider a simple generalization of the biaxial spin system in 1(a), and describe a pair of such spins by the Hamiltonian

$$\left.\begin{aligned} \mathcal{H}_0(\underline{S}_1,\underline{S}_2) &= \mathcal{H}_0(\underline{S}_1) + \mathcal{H}_0(\underline{S}_2) + V_0(\underline{S}_1,\underline{S}_2) \\ \text{where} \quad \mathcal{H}_0(\underline{S}_\mu) &= \frac{\hbar}{S_\mu}\left\{-\bar{K}_z^\mu \hat{S}_z^2 + \tfrac{1}{2}K_\perp^\mu\left[(S_\mu^+)^2 + (S_\mu^-)^2\right]\right\} \end{aligned}\right\} \quad (18)$$

$$\text{and} \quad V_0(\underline{S}_1,\underline{S}_2) = \mathcal{J}\,\underline{S}_1\cdot\underline{S}_2 + \underline{\mathcal{D}}\cdot(\underline{S}_1\times\underline{S}_2) \quad (19)$$

The form of $V_0(S_1,S_2)$ is not the most general - for example, the exchange term can be anisotropic, of form $J_{\alpha\beta}S_1^\alpha S_2^\beta$. There are also other possible terms. The DM interaction can only exist if there is a lack of inversion symmetry in the underlying system which hosts the 2 spins. Typically this would imply that the Hamiltonians $\mathcal{H}_0(\underline{S}_\mu)$ were different for the 2 spins, but we will assume they are the same, for simplicity. We will also assume that $|\underline{S}_1| = |\underline{S}_2| = \hbar S$, and write the interaction as

$$V_0(\underline{S}_1,\underline{S}_2) = \frac{\hbar}{S}\left\{\bar{J}\,\underline{S}_1\cdot\underline{S}_2 + \bar{\underline{D}}\cdot(\underline{S}_1\times\underline{S}_2)\right\} \quad (20)$$

with the classical version being given by a rather complex trigonometric expression which we do not write here.

It is clear that by switching on $\bar{J}$, we correlate the motion of the two spins; if $|\bar{J}| \gg |\bar{K}^z|, |\bar{K}^\perp|$, then the spins will be locked into parallel motion (if $\bar{J}$ is negative) or antiparallel motion (if $\bar{J}$ is positive). Clearly one can also mess around with the tunneling in very interesting ways with this exchange coupling - we discuss this later in some detail.

The effect of the DM (Dzyaloshinskii - Moriya) interaction is less obvious. Classically, it tries to force $\underline{S}_1$ and $\underline{S}_2$ to be perpendicular, with their cross-product anti-parallel to $\bar{\underline{D}}$. Quantum mechanically things are less obvious - the results (insofar as we know them) turn out to be very interesting.

A very interesting question that arises in all of this discussion is - how do entanglement properties appear in all of this? Clearly, since a path integral description of the spin pair is completely general, it must be encoded in the correlations between the paths - but how does this behave as one goes to a semiclassical regime? And how does entanglement affect the pairwise tunneling of the spins (which must now involve correlation between the tunneling events). To answer these questions, we need some tools:

2. SIMPLE METHODS

The 2 most obvious methods to employ in discussing spin tunneling are (i) WKB methods (which for spin tunneling have some interesting features), and (ii) straightforward perturbation theory. The way in which these 2 methods can be related is quite fascinating, and often unexpected.
An extra bonus is that the Hilbert space of the problem is rather small, which means that one is able to both explore and test quite fundamental and subtle ideas about non-perturbative effects, and on the spin path integral, using exact diagonalisation or other numerical methods.

2.1. PERTURBATION METHODS

At first glance it seems surprising that we could learn anything about a tunneling problem from perturbation theory. This is because we expect tunneling to be an intrinsically non-perturbative process. If we switch on a weak interaction $V(\epsilon) \sim \epsilon V_0$, which when added to a Hamiltonian $\mathcal{H}_0$ which does not allow tunneling, enables weak tunneling to take place, then we expect the tunneling amplitude to be $\sim O(\exp[-C_0/\epsilon])$, rather than being expandable as a power series in ϵ; tunneling should then be beyond any perturbative expansion (in a way similar to the non-perturbative nature of transitions in the adiabatic limit).
However the spin problem is unusual - one can actually calculate tunneling amplitudes using perturbation methods, and compare them with a non-perturbative calculation. Neither gives exact answers, as one can see by comparing with exact diagonalisation results.
The reason for this has mostly to do with the finite Hilbert space of the system, but some peculiarities caused by spin also enter the problem.
In what follows a very simple introduction is given to the use of perturbative methods for spin problems, since they are elementary; we then go on to do the same for WKB/instanton methods, and compare the two.

2.1.(a) FORMULATION of PERTURBATION EXPANSION

: Suppose we have a simple tunneling problem, in which a Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V}_0 = -D_0 \hat{S}_z^2 - \gamma \underline{S}\cdot\underline{H}_0^{\perp} \equiv -D_0 \hat{S}_z^2 - \underline{B}_0^{\perp}\cdot\underline{S} \equiv -t_1\left[\frac{k_z}{S}\hat{S}_z^2 + \underline{b}_0^{\perp}\cdot\underline{S}\right] \qquad (1)$$

is initially diagonalized in the basis $|S, M\rangle \equiv |M\rangle$ of eigenstates of $\mathcal{H}_0$, so that

$$\mathcal{H}_0 |M\rangle = -D_0 \hat{S}_z^2 |M\rangle = -D_0 M^2 \equiv E_0(M) \qquad (2)$$

We now wish to calculate the effects of the transverse field perturbatively, making an expansion in the dimensionless parameter $B_0/D_0 \equiv b_0 S/k_z$. To do this we first recall the basic formulae for spin matrix elements (cf. Appendix on spin representations):

$$\langle M+1|\hat{S}_+|M\rangle = \langle M|\hat{S}_-|M+1\rangle = [(S+M+1)(S-M)]^{1/2} \qquad (3)$$

so that

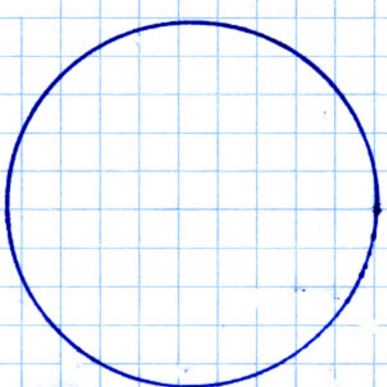
$$\left.\begin{aligned} \langle M+1|\hat{S}_x|M\rangle &= \langle M|S_x|M+1\rangle = \tfrac{1}{2}[(S+M+1)(S-M)]^{1/2} \\ \langle M+1|\hat{S}_y|M\rangle &= -\langle M|S_y|M+1\rangle = -\tfrac{i}{2}[(S+M+1)(S-M)]^{1/2} \end{aligned}\right\} \qquad (4)$$

For simplicity we will then take the field along the $\hat{x}$-axis, so that we can now view the problem in 2 quite complementary ways, as we see from the Figures below.

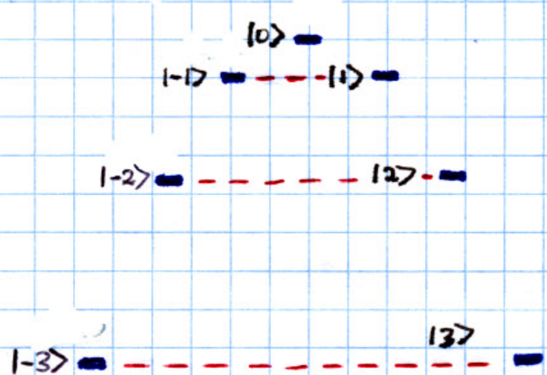
The first of these shows the classical potential created by applying the field to the system - here we assume a weak field, consistent with our assumption that

$$b_0/D_0 \ll 1 \qquad (5)$$

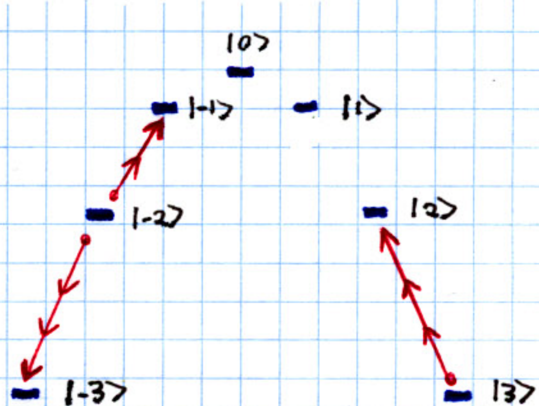
The form of this potential is of no obvious help in understanding the problem. However a diagram of the energy level structure in the basis $|M\rangle$ shows the key role of degenerate levels (see left); and the system has a "discretized barrier" form:



THE POTENTIAL $\mathcal{H}_0(S) = -D_0 S_z^2 - B_0 S_x$



PAIRS OF DEGENERATE STATES $|\pm M\rangle$



TYPICAL TRANSITIONS DRIVEN BY $\hat{S}_x$

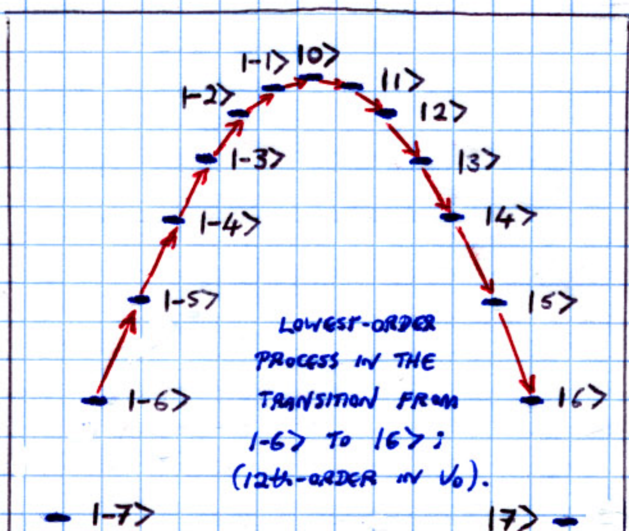
then one the right we see some of the transitions that can take place under the influence of the $\hat{S}_x$ operator. Consider now a pair of degenerate levels, ie., states $|M\rangle$ and $|-M\rangle$. These are connected in perturbation theory by a sequence of such transitions. The splitting between the levels is then given by the sum of all terms connecting the 2 levels. The first (lowest order in $\hat{S}_x$) sequence that contributes is the direct one, involving $2M$ transitions - it creates a pair of levels, of form

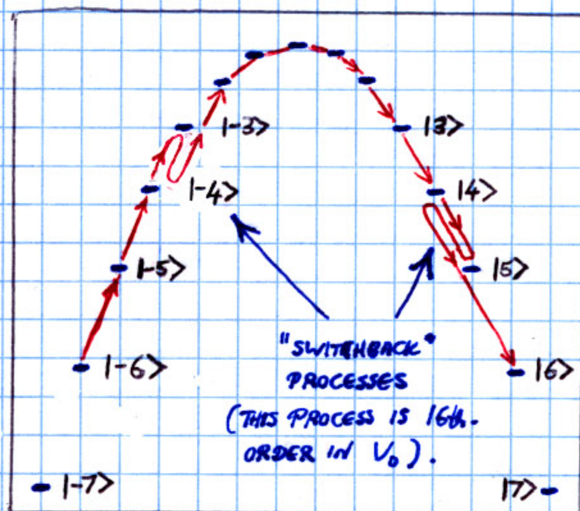
$$\left.\begin{aligned} |Sym\rangle_M &= \frac{1}{\sqrt{2}}\left(|M\rangle + |-M\rangle\right) \\ |AnS\rangle_M &= \frac{1}{\sqrt{2}}\left(|M\rangle - |-M\rangle\right) \end{aligned}\right\} \qquad (6)$$

which are shifted up/down by an energy $\frac{1}{2}\Delta_M$, where Δ_M is the splitting. Applying $\hat{S}_x$ to the state $|M-1\rangle$ a sequence of $2M$ times, we get

$$\left.\begin{aligned} \Delta_M = 2\left\{ \frac{V_0^{-M,-(M-1)}}{E^0_{-(M-1)} - E^0_{-M}} \times \cdots \times \frac{V_0^{M-2,M-1}}{E^0_{M-2} - E^0_M} \times \frac{V_0^{M-1,M}}{E^0_{M-1} - E^0_M} \right\} \\ + O\left(V_0^{2M+2}\right) \end{aligned}\right\} \qquad (7)$$

where the higher-order terms come from processes in which the system retraces its path one or more times (see Figure):





The matrix element in (7) is

$$V_0^{M+1,M} = \langle M+1|\hat{V}_0|M\rangle = \frac{1}{2}B_0\left[(S-M)(S+M+1)\right]^{1/2} \qquad (8)$$

and so we find

$$\Delta_M = 2D_0\left(\frac{B_0}{2D_0}\right)^{2M} \prod_{\ell=-M+1}^{M-1} \frac{1}{M^2-\ell^2} \prod_{\ell'=-M}^{M-1} \left[(S-\ell')(S+\ell'+1)\right]^{1/2} \qquad (9)$$

These products are evaluated in a straightforward way, and we get

$$\Delta_M = A^S_M D_0 \left[\left(\frac{B_0}{2D_0} \right)^{2M} + O\left(\frac{B_0}{2D_0} \right)^{2M+2} \right] \qquad (10)$$

where the prefactor is

$$A^S_M = \frac{2}{[(2M-1)!]^2} \frac{(S+M)!}{(S-M)!} \qquad (11)$$

The most interesting special case of this result is the splitting between the 2 lowest levels ($M=S$); we get

$$\Delta_S = \frac{4S(2S+1)}{(2S-1)!} D_0 \left(\frac{B_0}{2D_0} \right)^{2S} + \text{etc.} \qquad (12)$$

These expressions are not terribly illuminating at first glance. However let us consider the large S limit of (12). Using Stirling's formula, viz, that

$$\Gamma(n+1) = n! \sim (2\pi n)^{1/2} \left(\frac{n}{e} \right)^n \qquad (13)$$

we find that

$$\Delta_S \xrightarrow[S \gg 1]{} \frac{4}{\sqrt{\pi}} D_0 S^{3/2} \left(\frac{e B_0}{4 S D_0} \right)^{2S} \qquad (14)$$

so that

$$\ln \frac{\Delta_S}{D_0} \underset{S \gg 1}{\sim} \tfrac{3}{2} \ln S - 2S \ln \left(\frac{S D_0}{B_0} \right) \qquad (15)$$

Now this expression strongly suggests a WKB-style expression for the spin tunneling rate, of form

$$\left. \begin{aligned} & \Delta_S \sim A_S e^{-\Gamma_S^M} \\ \text{where} \quad & A_S \sim D_0 S^{3/2} \equiv \hbar \tilde{\omega}_2 S^{1/2} \\ \text{and} \quad & \Gamma_S^M \sim 2S \ln \left(\frac{S D_0}{B_0} \right) \end{aligned} \right\} \qquad (16)$$

A proper discussion of the relation between this perturbative result and the WKB / instanton results requires some care - we come to this later on.

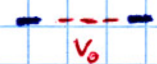
For completeness, note that we can also use Stirling's approximation to give a result for Δ_M in the case where both $S-M \gg 1$ and $M \gg 1$ (ie., for highly excited levels which are not too near the top of the "potential barrier" around $|M| \to 0$). In this intermediate tunneling regime one has the expression (next page):

$$\Delta_M \underset{\substack{S-M \gg 1 \\ M \gg 1}}{\sim} \frac{2}{\pi} D_0 \frac{(S+M)^{S+M+1/2}}{(S-M)^{S+M-1/2}} M \frac{e^{2M}}{(2M)^{4M}} \left(\frac{B_0}{2D_0}\right)^{2M} \qquad (17)$$

which can also be compared with a WKB calculation - we discuss this later.

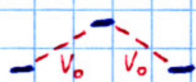
It is also interesting to consider these results for small S and M, where we can compare with exact analytic results very quickly. The lowest-order perturbative results for $S = 1/2, 1, 3/2$, and 2 are as follows:

- $S = 1/2$ (where $\mathcal{H}_0 = 0$): $\Delta_{1/2} = V_0^{1/2,-1/2} = B_0$ (18)



This is of course the correct and exact result.

- $S = 1$: Here we have $\Delta_1 = \dfrac{|V_0^{01}|^2}{E_0 - E_1} = \dfrac{B_0^2}{D_0}$ (19)



This result is not exact - it is an approximation to the correct expression

$$\Delta_1 = \tfrac{1}{2} D_0 \left[\sqrt{1 - 4B_0^2/D_0^2} - 1\right] \qquad (20)$$

in the limit $B_0 \ll D_0$. The reason of course is that (19) only includes the lowest 2nd-order process, and ignores 4th, 6th, 8th, etc order processes in which the spin quantum number M undergoes "switchback" processes.

- $S = 3/2$: Here we have

$$\left.\begin{aligned} \Delta_{3/2} &= \frac{3}{8} \frac{B_0^3}{D_0^2} \\ \Delta_{1/2} &= 2 B_0 \end{aligned}\right\} S = 3/2 \qquad (21)$$

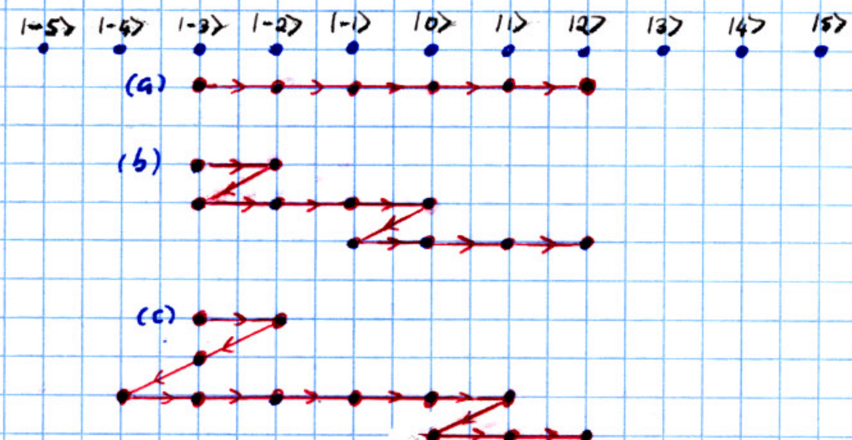
- $S = 2$: Here we have

$$\left.\begin{aligned} \Delta_2 &= \frac{1}{12} B_0^4/D_0^3 \\ \Delta_1 &= 3 \frac{B_0^2}{D_0} \end{aligned}\right\} S = 2 \qquad (22)$$

and so on. We notice that the results for Δ_1 are not these same for $S = 1$ and $S = 2$. Mathematically this is because of the factors in (3) and (4) in the matrix elements. Physically we see that the presence of the extra levels and the larger Hilbert space in the case $S=2$ actually enhances Δ_1 over the value when $S=1$.

The disparity between the exact results and the lowest-order perturbative result, coming from the higher-order "switchback" processes, is of some interest in the context of field theory, and of the mathematics of asymptotic series. For large S we can think of these switchback processes as sub-dominant contributions to the leading-order term, which itself can be brought into correspondence with the WKB result. We discuss all of this later on.

Finally, this example brings out nicely the way in which the perturbation expansion simply labels the different paths in a "discretized" path integral - inevitably discretized because the Hilbert space itself is finite. We show this for the same problem as above (here for $S=5$):



All of the above processes involve the propagation of the system from the state $|-3\rangle$ to $|2\rangle$. Thus they are all processes contributing to the Green function

$$G_{2,-3}(t) = \langle 2 | \hat{G}(t) | -3 \rangle \qquad (23)$$

The process (a) is a direct process, $\sim O(B_0^5/D_0^4)$. The process (b) is a switchback process $\sim O(B_0^9/D_0^8)$. The process (c) is another switchback process, this time of order $\sim O(B_0^{11}/D_0^{10})$; notice that it now involves an excursion back to state $|-4\rangle$, further to the left than the originating state $|-3\rangle$.

We develop this perturbative calculation for $G_{MM'}(t)$ with more systematic rigour later on. Before doing this it is helpful to consider a few examples of tunneling problems, treated by perturbation theory, since the example just considered does not display all the interesting features of this method, or the results one gets from it.