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Metastable lifetimes, level crossings and vertical cuts in quantum mechanics

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Abstract. We illustrate the relationship between square-root branch points of energy eigenvalues and the decay rates of metastable states in a simple model in quantum mechanics involving decay through a delta-function potential barrier. The 'infinite volume' limit of the cut-structure is found to have an interesting pathology.

1. Introduction

There has been interest in recent years in the decay of metastable states in quantum and statistical physics (see reference list). The analytic structure of energy eigenvalues as a function of parameters of the theory plays an important role in such problems. This article is concerned with the decay rate in quantum mechanics of metastable states in a potential of the form illustrated in figure 1. Our aim is to link the following two approaches to this problem.

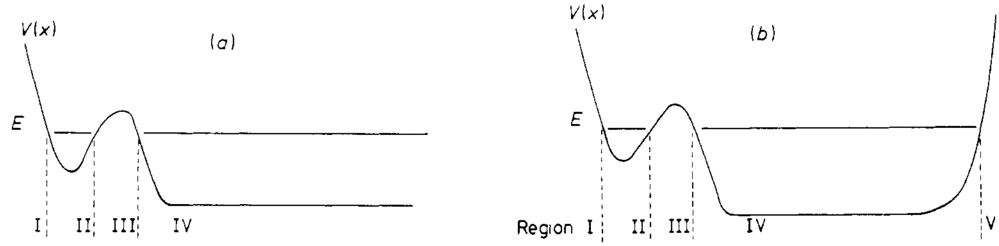

Figure 1. Form of potential admitting metastable states.

One standard approach looks for stationary states (i.e. not necessarily normalisable functions ψ satisfying $H\psi = E\psi$) which satisfy the outgoing wave boundary conditions in region IV and tend to zero in region I (of figure 1(a)). The calculation

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can be done for an arbitrary potential function V using for example the WKB approximation. The resulting equations imply that the allowed eigenvalues E must be complex, with the (negative) imaginary part of E related to the decay rate of the metastable state initially localised in region II.

A second approach starts from a 'finite volume' system in which the region into which the metastable state decays is of large but finite extent (see figure 1(*b*)). One looks for normalisable energy eigenstates requiring that the wavefunction vanish in regions I and V. In this case, the Hamiltonian is self-adjoint and energy eigenvalues are correspondingly real. For energy levels not too close to the top of the potential barrier in region III there is little tunnelling and the spectrum is close to that of two disconnected potential wells one of which is very wide. This is illustrated in figure 2.

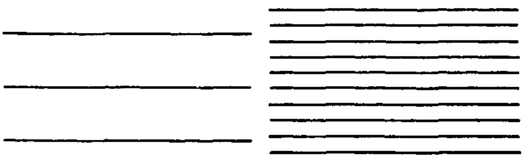

Figure 2. Qualitative spectrum for potential as in figure 1. The wide potential well gives rise to a closely spaced spectrum; the extra states are localised in the metastable region if the potential barrier is large.

The most important corrections to this naive spectrum occur when two levels are very close together. This is related to the phenomenon of level crossing which occurs as, say, the height h of the metastable potential well is varied, and which gives rise to pairs of complex conjugate branch points (in the complex h plane) which can be connected by vertical branch cuts. That this is true can be seen by taking a 2×2 matrix representation of the Hamiltonian with respect to the two almost degenerate states. This takes the form

$$\begin{pmatrix} h & \epsilon \\ \epsilon & -h \end{pmatrix}$$

where the level crossing occurs at $h=0$ and ϵ represents the (small) overlap between the states due to the tunnelling effect. The eigenvalues of this matrix are

$$E = \pm\sqrt{(h^2+\epsilon^2)} \tag{1}$$

which shows the branch points in energy as a function of complex h to be at $h=\pm\mathrm{i}\epsilon$. The two branches in (1) can be represented in the two-sheeted complex h plane cut from $+\mathrm{i}\epsilon$ to $-\mathrm{i}\epsilon$. If the cuts are placed from $\mathrm{i}\epsilon\to\mathrm{i}\infty$ and $-\mathrm{i}\epsilon\to-\infty$, we can obtain on the first sheet the eigenvalue of the ground state and on the second sheet the eigenvalue of the higher energy state. If we wish to obtain a description of a metastable state which starts as the ground state for $h<0$, say, and survives to become the excited state for $h>0$, we go from one branch of the square root in (1) to the other. This is achieved by placing the cut between the points $\pm\mathrm{i}\epsilon$. Analytic continuation to the metastable state can be done only by going round the branch cuts.

The physical basis for this description of metastability is that for large h, away from the level crossing, the system is described by the *same* state (the eigenvector $(1,0)$) both for $h<0$ *and* $h>0$, i.e. the state of the system is almost unchanged by the level crossing. The metastable state is traced because it remains essentially unchanged through the level crossings. (From the standpoint of time-dependent perturbation theory this is the 'sudden approximation'. In the opposite extreme—the 'adiabatic approximation'—the state label is unchanged. Interestingly, corrections to the adiabatic approximation, i.e. label changing transitions, can be computed by contour integrals around vertical cuts (Landau and Lifshitz 1965), but we emphasise that although vertical cuts between level-crossing branch points play a role in both calculations the underlying physics is different. In particular the distance of branch point into the complex plane reflects the rate of the process, being small in our case and large for the Landau–Lifshitz calculation.)

The sequence of level crossings suffered by a metastable state as the height h of the metastable potential is varied implies that a metastable energy level is analytic in the cut h plane as shown in figure 3. The importance of vertical cuts in the description of metastability in the Ising model is discussed by Newman and Schulman (1977) and by McCraw and Schulman (1978). In the present paper, we wish to show in a simple model in quantum mechanics how these vertical cuts condense, for large volume, to reproduce the imaginary part of E (and hence the lifetime) encountered in the first type of calculation outlined above.

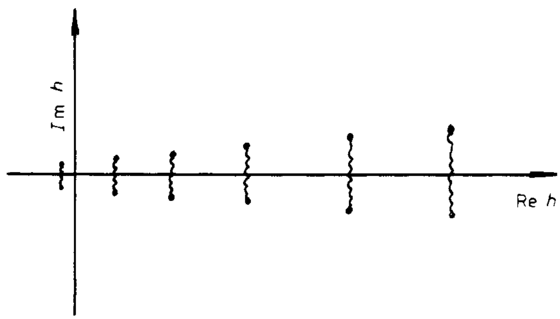

Figure 3. Cut structure for a metastable level in the complex h plane.

We also show that when the volume increases beyond a certain size the branch cut structure is lost but the analytic continuation of the finite volume energy level continues to give the lifetime even though the underlying quantum mechanics problem no longer yields the analytically continued energy. In effect the limits [volume $\to \infty$] and [(complex h)$\to$(real h)] do not commute. This will be illustrated below.

2. Calculation

The potential we choose is shown in figure 4. In the allowed region the Hamiltonian (in suitable units) has the form

$$H = p^2 - h\epsilon(x) + \lambda\delta(x), \qquad \epsilon(x) = \begin{cases} +1 & x > 0 \\ -1 & x < 0. \end{cases} \tag{2}$$

Thus $2h$ is the height of the metastable potential and the delta function potential barrier has strength λ. The size of the metastable well is a, and the stable well b, so that boundary conditions $\psi(-a) = \psi(b) = 0$ are imposed. We are interested in $b \gg a$.

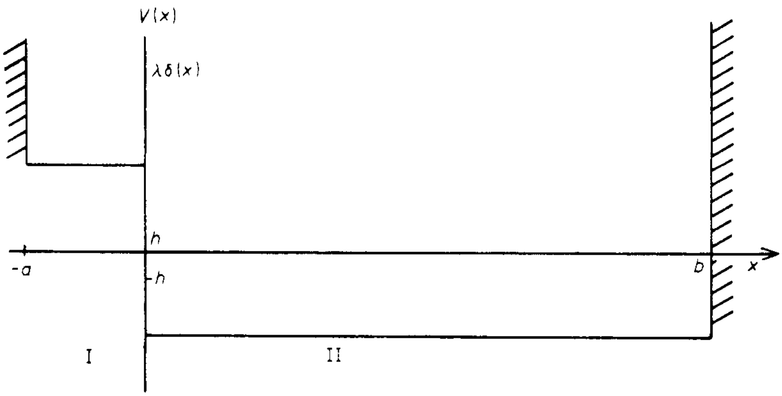

Figure 4. Potential for simple model calculation. Region I is $x<0$. Region II is $x>0$.

For the calculation of the metastable lifetime we first use the method described above in which '$b=\infty$' and we allow only outgoing waves in region II. The wavefunctions take the form

$$\psi_{\mathrm{I}}(x)=\sin k(x+a), \qquad x<0, \quad k^2=E-h$$
$$\psi_{\mathrm{II}}(x)=B\,\mathrm{e}^{\mathrm{i}lx}, \qquad x>0, \quad l^2=E+h$$

where E is the energy of the state. The δ-function imposes a discontinuity in ψ' at $x=0$ and the equation for E (or k and l) is

$$-k\cot ka+\mathrm{i}l-\lambda=0. \tag{3}$$

For large λ (i.e. small tunnelling) we can neglect the imaginary term in this equation and the values of k are close to the zeros of $\sin ka$. (This gives the energy levels in well I if there is no tunnelling into II.) In this region we can make the replacement

$$k\cot ka\sim k/(ka-\pi) \tag{4}$$

for the lowest metastable state (excited states can be similarly treated). The resulting equation yields

$$E-h=\frac{\pi^2}{(a+1/\lambda)^2}-\frac{2\mathrm{i}\pi^2}{\lambda^2a^3}\left(2h+\frac{\pi^2}{a^2}\right)^{1/2}+\mathrm{O}(1/\lambda^3). \tag{5}$$

The negative imaginary part in E gives rise to a decaying amplitude for the metastable state with decay rate

$$\frac{1}{\tau}=\frac{4\pi^2}{\lambda^2a^3}\left(2h+\frac{\pi^2}{a^2}\right)^{1/2}+\mathrm{O}(1/\lambda^3).$$

We now show how the imaginary part in (5) is reproduced in a 'finite volume' calculation with wavefunctions

$$\begin{aligned}\psi_{\mathrm{I}}(x)&=A\sin k(x+a), \qquad x<0, \quad k^2=E-h\\ \psi_{\mathrm{II}}(x)&=B\sin l(x-b), \qquad x>0, \quad l^2=E+h.\end{aligned} \tag{6}$$

The eigenvalue condition analogous to (3) is now

$$k\cot ka+l\cot lb+\lambda=0. \tag{7}$$

For large λ, the eigenstates have eigenvalues close to those determined either by $\sin ka \sim 0$ (wavefunction localised in the metastable region) or by $\sin lb \sim 0$ (wavefunction localised in the stable region). The level crossings which give rise to the vertical cuts occur for values of h for which both $\sin ka \sim 0$ and $\sin lb \sim 0$ for large λ.

The location of the branch points due to the level crossings can be obtained analytically for large λ by making the approximations $\cot ka \sim (ka - \pi)^{-1}$ and $\cot lb \sim (lb - j\pi)^{-1}$. This corresponds to the crossing of the first metastable state with jth level in region II. Expression (7) then becomes

$$kl + \alpha k + \beta l + \gamma = 0 \tag{8}$$

where

$$\alpha = -j\pi(1 + \lambda a)/(b + a + \lambda ab) \tag{9a}$$

$$\beta = -\pi(1 + \lambda b)/(b + a + \lambda ab) \tag{9b}$$

$$\gamma = \lambda j\pi^2/(b + a + \lambda ab). \tag{9c}$$

Squaring equation (8) gives

$$k^2 l^2 = \alpha^2 k^2 + \beta^2 l^2 - \gamma^2 + 2(\alpha\beta - \gamma)kl. \tag{10}$$

For large λ, equation (9) shows that α, β and γ are $O(1)$, while $\alpha\beta - \gamma = O(1/\lambda^2 b)$. Although it turns out that this fact is not sufficient to justify the neglect of the kl term in equation (10), it does allow a derivation based on successive approximation. We therefore define

$$\rho^2 = \gamma^2 - 2kl(\alpha\beta - \gamma) = \gamma^2 - \epsilon.$$

Using the definitions of k^2 and l^2, equation (10) becomes a quadratic equation for the two eigenvalues in the level crossing region and we find

$$E = \tfrac{1}{2}(\alpha^2 + \beta^2) \pm \tfrac{1}{2}[(2h - \alpha^2 + \beta^2)^2 + 4(\alpha^2\beta^2 - \rho^2)]^{1/2}.$$

In factoring $\alpha^2\beta^2 - \rho^2$, the term $\alpha\beta + \rho$ can be well approximated by $\alpha\beta + \gamma$. However, in dealing with $\alpha\beta - \rho$ a subtle reappearance of an ostensibly negligible term occurs:

$$\alpha\beta - \rho = \alpha\beta - \surd(\gamma^2 - \epsilon) = \alpha\beta - \gamma + \frac{\epsilon}{2\gamma} + O(\epsilon^2/\gamma^3).$$

The quantity ϵ is proportional to $\alpha\beta - \gamma$ and we obtain

$$\alpha\beta - \rho = (\alpha\beta - \gamma)\left(1 + \frac{kl}{\gamma}\right).$$

Now k and l differ from π/a and $j\pi/b$ respectively by terms of order $1/\lambda$ and keeping only lowest order terms in $1/\lambda$

$$\alpha\beta - \rho = 2(\alpha\beta - \gamma).$$

The expression for E is therefore

$$E = \tfrac{1}{2}(\alpha^2 + \beta^2) \pm \tfrac{1}{2}[(2h - \alpha^2 + \beta^2)^2 + 8(\alpha^2\beta^2 - \gamma^2)]^{1/2}. \tag{11}$$

The discriminant has been written so that it is easy to see that the degeneracy of the jth level crossing occurs at

$$h = h_j \pm \mathrm{i}\tau_j$$

where

$$h_j = \pi^2(j^2/b^2 - 1/a^2)/2 + \mathrm{O}(1/\lambda) \tag{12a}$$

$$\tau_j = \frac{2j\pi^2}{\lambda b^{3/2} a^{3/2}}[1 + \mathrm{O}(1/\lambda)]. \tag{12b}$$

(We need these expressions only to leading order in $1/\lambda$ to obtain the imaginary part in equation (5)).

Thus the jth level crossing gives rise to a vertical cut between $h = h_j \pm \mathrm{i}\tau_j$ and the discontinuity of E across this cut,

$$\Delta E = 2[(h - h_j)^2 + \tau_j^2]^{1/2}, \tag{13}$$

is real. Both the spacing and the height of the cuts shrink for large b, according to equation (12). One may smear their effect by means of a dispersion relation. If we take a contour C enveloping the vertical cuts we can evaluate it by summing the integrated discontinuities across each cut as in figure 5. Note that the contributions are pure imaginary since the discontinuities are pure real. A simple calculation yields

$$E(h) = \frac{1}{2\pi \mathrm{i}} \int_C \frac{E(h')\,\mathrm{d}h'}{h' - h} = -\frac{2}{\pi}\sum_j \int_0^{\tau_j} \mathrm{d}\tau \frac{\sqrt{(\tau_j^2 - \tau^2)}}{h_j + \mathrm{i}\tau_j - h} = -\tfrac{1}{2}\sum_j \frac{\tau_j^2}{h_j - h} \tag{14}$$

where the integration variable τ is defined by $h' = h_j + \mathrm{i}\tau$ and the expression (14) is correct only to leading order in τ_j as required for large b. For large b, the sum on j can be replaced by an integral on the variable h'' (cf equation (12a))

$$h'' = \frac{\pi^2}{2}\left(\frac{j^2}{b^2} - \frac{1}{a^2}\right)$$

and one obtains

$$E(h) = -\frac{2\pi}{\lambda^2 a^3} \int \mathrm{d}h'' \frac{\sqrt{(2h'' + \pi^2/a^2)}}{h'' - h}. \tag{15}$$

This equation has the form of a dispersion relation with the original contour C in figure 5. It implies that for large b the vertical cuts reproduce the effect of a cut *along* the h axis, in which the discontinuity comes from an imaginary part

$$\mathrm{Im}\, E = -\frac{2\pi^2}{\lambda^2 a^3}\left(2h + \frac{\pi^2}{a^2}\right)^{1/2} \tag{16}$$

exactly as in equation (5).

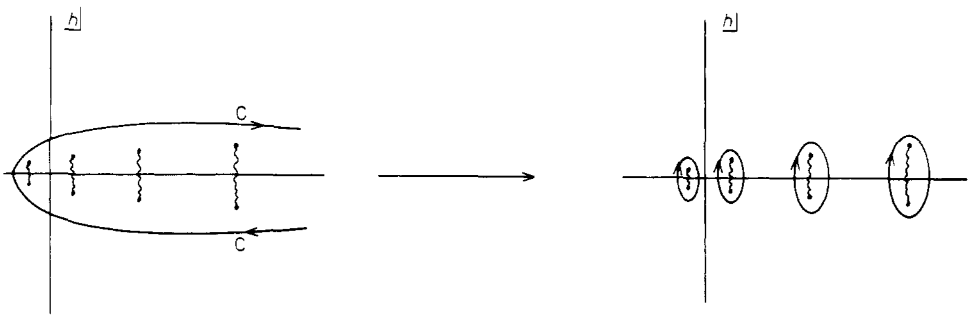

Figure 5. Deformation of the integration contour C in the dispersion relation.

The apparent divergence of the integral in equation (15) is no problem since what one actually ought to be using is a twice subtracted dispersion relation ($E(h) \sim h +$ constant$+\ldots$). All our conclusions remain valid when the convergent form is used and so we spare the reader the additional calculations.

It may be worth pointing out the distinction between what is going on in the E plane and in the h plane. In the E plane the energy value obtained in (5) is a pole in the Green function on the unphysical sheet (a 'stationary state' with unphysical boundary conditions) and hence sits well with the traditional picture of metastability in quantum mechanics. On the other hand, *as an analytic function of h, $E(h)$* is analytic (and single valued) in the entire half plane $\operatorname{Re} h < -\pi^2/2a^2$. However, at $h = -\pi^2/2a^2$ there is a branch point, evident from equation (5). For the dispersion relation contemplated above the branch cut is assumed to run along the real h axis, $\operatorname{Re} h > -\pi^2/2a^2$. Taking $E(h)$ for $\operatorname{Im} h > 0$ to be as given in equation (15), $E(h)$ in the lower half plane will just be its complex conjugate and the discontinuity is, as usual, twice the imaginary part.

Although it may not be obvious, our calculations up to this point hold only for $b \ll \lambda^2 a^3$, so that although for large λ setting sums equal to integrals (as we have done) is not invalidated, nevertheless, for the limit $b \to \infty$, λ fixed, our conclusions are not true. Before writing formulae valid for *very* large b we first indicate why the condition $b \ll \lambda^2 a^3$ is physically reasonable in the context of our previous discussion and point out where in our calculations that condition was implicitly assumed. First introduce some notation. Let E_∞ represent the solution of equation (3), given approximately by equation (5). Let E_b be the solution to equation (7).

For $k \sim \pi/a$ the metastable state is supposed to be localised mainly in the region $x < 0$ with slight leakage into $x > 0$. Only under these circumstances would E_b (for h real and positive) be expected to equal E_∞. But the wavefunction leakage through the barrier (i.e. the ratio B/A of equation (6)) is proportional to $1/\lambda a$. Hence the total probability for being found in $x > 0$ is $b/\lambda^2 a^2$, while the probability to be in $x < 0$ is $\mathrm{O}(a)$. From this follows the condition $b/\lambda^2 \ll a^3$. This condition also plays a role in our assumption that the level $k \sim \pi/a$ 'interacts' with only one level of the region $x > 0$ at a time. For this to be true one would expect the distance of the branch points from the real axis to be small compared to the spacing between levels. The solution equation (12) gives this condition as

$$\frac{2\pi^2 j}{\lambda b^{3/2} a^{3/2}} \ll \frac{2\pi^2 j}{b^2}, \qquad \text{i.e.} \quad b \ll \lambda^2 a^3.$$

Our implicit use of the condition $\lambda^2 \gg b/a^3$ occurred in assuming $|lb - j\pi| \ll 1$, preliminary to deriving equation (8). That equation ultimately yielded a branch point at $h = h_j \pm \mathrm{i}\tau_j$ so that $\operatorname{Im} l \sim \tau_j \sim 1/\lambda b^{1/2} a^{3/2}$. (Note that $j/b = \mathrm{O}(1)$.) Consequently, for the branch point $|lb - j\pi| \geq b|\operatorname{Im} l| \sim (b/\lambda^2 a^3)^{1/2}$ and the assumption used in expanding the cotangent breaks down unless the condition $\lambda^2 a^3 \gg b$ is satisfied.

To find formulae for branch points valid for all b we use a more general method. Let

$$F(E, h) \equiv k \cot ka + l \cot lb + \lambda \tag{17}$$

with k and l defined in terms of E and h, as in (6). The function $E(h)$ is of course defined by $F(E, h) \equiv 0$. Branch points will occur when, in addition, $\partial F/\partial E = 0$. This can be written

$$\frac{1}{k}\cot ka+\frac{1}{l}\cot lb-\left(\frac{a}{\sin^2 ka}+\frac{b}{\sin^2 bl}\right)=0. \tag{18}$$

If we were to assume $|bl-j\pi|\ll 1$ here, $\sin^2 bl$ could be replaced by $(bl-j\pi)^2$ and we would return to our previous results. But we now consider the opposite extreme and note that to nullify the b in the parentheses we must have $\sin^2 bl\to\infty$, which requires l to have a small imaginary part. Looking now at $b\gg\lambda^2a^3$ we have in fact ($l=l_1+il_2$)

$$l_2\sim\pm(\ln b)/2b. \tag{19}$$

For this l_2, $\cot bl\sim -\mathrm{i}\,\mathrm{sgn}(l_2)$ so that at the branch point we must have

$$k\cot ka-\mathrm{i}l\,\mathrm{sgn}\,(l_2)+\lambda=0 \tag{20}$$

which is the same as equation (3) for $l_2>0$, but with this difference in meaning: it is an equation to locate h_{B} (the value of the branch point) rather than provide E_∞ as a function of h. Nevertheless, from (20) we can still get the result of equation (5), so that (taking $\mathrm{sgn}(l_2)>0$)

$$\mathrm{Im}(E-h)=-\frac{2\pi^2}{\lambda^2a^3}\left(2h+\frac{\pi^2}{a^3}\right)^{1/2}. \tag{21}$$

Since $l^2=l_1^2-l_2^2+2\mathrm{i}l_1l_2=E+h$, adding $2h$ to equation (21) yields

$$\mathrm{O}\left(\frac{\ln b}{b}\right)=2l_1l_2=2\,\mathrm{Im}\,h_{\mathrm{B}}-\frac{2\pi^2}{\lambda^2a^3}\left(2h+\frac{\pi^2}{a^2}\right)^{1/2}. \tag{22}$$

For $b\to\infty$ this implies

$$\mathrm{Im}\,h_{\mathrm{B}}=\frac{\pi^2}{\lambda^2a^3}\left(2h+\frac{\pi^2}{a^2}\right)^{1/2}\sim\frac{\pi^2}{\lambda^2a^3}\left(2\,\mathrm{Re}\,h_{\mathrm{B}}+\frac{\pi^2}{a^2}\right)^{1/2}=\mathrm{O}\left(\frac{1}{\lambda^2}\right). \tag{23}$$

Thus we find branch points spaced $1/b$ apart, a distance $1/\lambda^2$ from the real h axis (contrast this to $\tau_j\sim 1/\lambda\sqrt{b}\,a^{3/2}$ for $b\ll\lambda^2a^3$). Hence E_b, near the real positive h axis seems to be showing bad behaviour.

Let us now go some distance into the complex h plane and turn some of these calculations around. Continue to assume that k never gets far from π/a. Then since $l^2=k^2+2h$, $\mathrm{Im}\,h>0$ implies $\mathrm{Im}\,l>0$, implies $\cot bl\sim -\mathrm{i}\,\mathrm{sgn}(l_2)$. Hence the equation for E_b becomes (almost) exactly the same as that for E_∞ in the upper half h plane, while in the lower half h plane it coincides (nearly) with an incoming wave version of equation (3) and it therefore nearly gives the same discontinuity as E_∞ across the real positive h axis. This happy situation obtains up until a distance $1/\lambda^2$ from the real h axis, where E_b, for any finite b, picks up all sorts of singularities while E_∞ shows no untoward behaviour at all.

Define $E_{\mathrm{L}}=\lim_{b\to\infty}E_b$. We have found that sufficiently far from the real positive h axis $E_{\mathrm{L}}=E_\infty$ but that for $|\mathrm{Im}\,h|<1/\lambda^2$ they differ. Since E_∞ is analytic it must be the case that the limit $b\to\infty$ sends E_b into several different functions†. Call the one that coincides with E_∞ well off the real positive h axis, $E_{\mathrm{L}1}$. We can ask whether $E_{\mathrm{L}1}$ can be analytically continued to the real positive h axis. The answer is, certainly, since $E_{\mathrm{L}1}$

† Function theory does not forbid this. Consider $[Z\exp(-bZ)+1]/[Z+\exp(-bZ)]$ for Re Z positive or negative. Another example is $F(Z)=\int_{-b}^{b}\exp(-Zx^2)\,\mathrm{d}x$, for which $F_{\mathrm{L}}=\lim_{b\to\infty}F(Z)$, Re $Z>0$, is $\sqrt{(\pi/Z)}$. F_{L} can be continued to Re $Z<0$ but is no longer given by the integral.

and E_∞ coincide elsewhere and E_∞ is defined on the real positive h axis. Call the analytically continued E_{L1}, $\tilde{E}$.

The amusing part is that although E_{L1} can be analytically continued to $\tilde{E}$, for h real and positive, $\tilde{E}$ no longer is the solution of any quantum mechanical boundary value problem. The difference between E_∞ and E_L arises from the term e^{-2lb} which though negligible in most of the complex h plane, becomes important for large enough b for real positive h.

3. Conclusion

For the simple model studied in this paper and for large but finite volume we have thus (through comparison of equations (5) and (16)) established our contention that the imaginary part of the energy which appears in the calculation of the decay rate of metastable states arises as a condensation of vertical cuts associated with level crossings. For any finite volume, the energy of a stationary state is real if the potential is real but the condensation of the vertical cuts mimics a cut (more descriptively, a tear) along the real axis with discontinuity precisely the imaginary part associated with the decay rate. A similar description can be given of metastability in the Ising model.

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