Barrier penetration via perturbation theory

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Abstract. It is shown that Fermi's golden rule is valid for any initial state having a very narrow energy spread, even if it is not an eigenstate of the 'free Hamiltonian'. As an example, we compute explicitly the tunnelling rate through a rectangular barrier. This method may have applications in the Stark effect, autoionisation, fission, and similar problems.

1. Formulation and solution of the problem

A familiar problem of quantum theory is the calculation of the energy levels and decay rates of metastable systems, such as in the Stark effect or the anharmonic oscillator. It is somewhat frustrating that the real part of the energy can be easily evaluated by perturbation theory, with reasonable accuracy, but its imaginary part (the decay rate) cannot, with a few exceptions (Benassi *et al* 1979).

The reason for this difficulty is the following. In the standard treatment, one writes $H = H_0 + V$ and H_0 is chosen in such a way that the equation $H_0 u_m = E_m u_m$ can be solved explicitly. The Schrödinger wavefunction is then written as

$$\psi = \sum a_m(t)u_m \exp(-iE_m t). \tag{1}$$

Moreover it is assumed that
  (a) the initial state ϕ is an eigenfunction of H_0, say u_0, and
  (b) in the Schrödinger equation

$$i\dot{a}_k = \sum V_{km} \exp[i(E_k - E_m)t]a_m \tag{2}$$

it is possible to neglect the product $V_{km}a_m$ for $k \neq 0 \neq m$. Here V_{km} denotes as usual the matrix element (u_k, Vu_m).

These two assumptions are usually incompatible. For example, consider the following barrier penetration problem:

$$H = \frac{-1}{2m} \frac{d^2}{dx^2} + V_0 + V_1 + V_2, \tag{3}$$

where V_0 is a positive constant and

$$V_1 = -V_0\theta(a - |x|), \tag{4}$$

$$V_2 = -V_0\theta(|x| - b). \tag{5}$$

Here θ denotes the unit step function and it is assumed that $b > a$,

$$ma^2 V_0 \gg 1, \tag{6}$$

and

$$m(b-a)^2 V_0 \gg 1, \tag{7}$$

i.e. we have a large potential well for $|x| < a$, surrounded by a thick and high barrier extending up to $|x| = b$. The particle is initially trapped in the well, e.g. ϕ may be the ground state of $H - V_2$. We are therefore tempted to identify $H_0 = H - V_2$, so that $V = V_2$.

Assumption (b) above thus implies that we can neglect all the matrix elements of V_2, except those related to the ground state of $H - V_2$. Now, if this were true, we could derive the golden rule in the usual fashion (Schiff 1949) but the latter would give a zero result, because $H - V_2$ (which plays the role of H_0) has no continuum of states in the vicinity of its ground state! Since we know that tunnelling is certainly possible, it appears that assumption (b) cannot hold with *this* choice of a_m: even though each term in the sum (2) is small, the latter may converge so slowly that it cannot be restricted to the $m = 0$ term.

It is not difficult to guess the cause of the trouble. The Hamiltonian H has indeed a continuum of eigenstates with energies close to E_0, but these states resemble more the eigenstates of $H - V_1$ than those of $H - V_2$. With these states as the basis and V_1 as the perturbation, the sum (2) should converge very well. We shall therefore identify $H_0 = H - V_1$ (rather than $H - V_2$). But then *the initial state ϕ is not an eigenstate of H_0.*

Another example, more realistic than (3), is autoionisation or resonant scattering of electrons by atoms (O'Malley and Geltman 1965, Miller 1966). Consider for instance the decay of an excited state of the helium atom: $He^* \to He^+ + e$. In this case, H_0 should represent the He^+ ion plus the kinetic energy of the outgoing electron, and the initial metastable state He^* is not at all an eigenstate of H_0.

Our task is to investigate the Schrödinger equation (2) under no other assumption than that *the initial state has a very small ΔH*. First, we note that

$$\sum V_{km} a_m \exp(-iE_m t) = \sum (u_k, V u_m)(u_m, \psi) = (u_k, V\psi), \tag{8}$$

so that the Schrödinger equation can be written (still exactly) as

$$i \dot{a}_k = (u_k, V\psi) \exp(iE_k t). \tag{9}$$

We now replace ψ, in the RHS of (9), by $\exp(-iE_0 t)\phi$, where $E_0 = (\phi, H\phi)$. This must be a good approximation, if ΔH is small. We thereby obtain

$$i \dot{a}_k = V_{k0} \exp[i(E_k - E_0)t], \tag{10}$$

where $V_{k0} = (u_k, V\phi)$. This result is valid to first order in V. Integration of (10) yields

$$a_k(t) = a_k(0) - V_{k0} \frac{\exp[i(E_k - E_0)t] - 1}{E_k - E_0}, \tag{11}$$

which can now be substituted back into the RHS of (2), giving $\dot{a}_k$ correct to second order in V:

$$i \dot{a}_k = \sum V_{km} \exp[i(E_k - E_m)t] \left\{ a_m(0) - V_{m0} \frac{\exp[i(E_m - E_0)t] - 1}{E_m - E_0} \right\}. \tag{12}$$

This in turn can be used to evaluate the decay rate

$$\Gamma = -\frac{\mathrm{d}}{\mathrm{d}t} \left| \sum \bar{a}_k(0)a_k \right|^2 \tag{13}$$

or

$$\Gamma \simeq -2 \operatorname{Re} \sum \bar{a}_k(0)\dot{a}_k, \tag{14}$$

the last expression being valid for $a_k \simeq a_k(0)$.

As V_{km} is Hermitian, the first term in the braces in (12) does not contribute to Γ. In the second term, the expression $\Sigma \bar{a}_k(0) V_{km}$ is simply $\bar{V}_{m0}$, because of (8), and we obtain

$$\Gamma = 2\sum |V_{m0}|^2 \sin[(E_m - E_0)t]/(E_m - E_0). \tag{15}$$

This result is similar to the one derived in elementary time-dependent perturbation theory (Schiff 1949) and again leads to Fermi's golden rule. The latter therefore remains valid even if the initial state is *not* an eigenstate of H_0, provided only that ΔH is very small. It is however essential to split H correctly into $H_0 + V$: some of the eigenstates of H_0 must resemble as much as possible the *final* state of our system (*after* the decay).

2. Example: tunnelling through a rectangular barrier

As an example, let us compute Γ for the barrier penetration problem defined by equations (3)–(7). The initial state ϕ will be the ground state of $H - V_2$. This is the standard one-dimensional square well. We write

$$\begin{aligned} \phi &= A \cos kx, & |x| &< a, \\ &= B \, \mathrm{e}^{-\kappa x}, & |x| &> a. \end{aligned} \tag{16}$$

The energy

$$E_0 = k^2/2m = V_0 - \kappa^2/2m \tag{17}$$

is found by requiring ϕ'/ϕ to be continuous at $x = a$. This gives

$$k \tan ka = \kappa, \tag{18}$$

whence $k \simeq \pi/2a$ and $A \simeq a^{-1/2}$, if (6) holds.

Likewise, the even eigenfunctions of $H_0 = H - V_1$ are

$$\begin{aligned} \psi &= C \cosh \kappa x, & |x| &< b, \\ &= D \cos(k|x| + \delta), & |x| &> b. \end{aligned} \tag{19}$$

Requiring ψ'/ψ to be continuous at $x = b$ yields

$$\kappa \tanh \kappa b = -k \tan(kb + \delta), \tag{20}$$

which is a relationship between δ and E. For the purpose of normalisation, it is convenient to enclose the system in a large 'box' $-L < x < L$, which makes the energy levels discrete. For example, we may assume that $\psi(-L) = \psi(L) = 0$ and get, besides (20),

$$kL + \delta = (n + \tfrac{1}{2})\pi \tag{21}$$

where n is an integer. Now, for $L \gg b$, the energy levels are very closely spaced and equation (20) shows that δ, which is a continuous function of E, will change very little from one level to the next. Consecutive energy levels thus have $\Delta k \simeq \pi/L$ and there are

$$\rho(E)dE = (m/2E)^{1/2}(L/\pi)dE \tag{22}$$

energy levels between E and $E + dE$. It is readily seen that the normalisation constant is $D \simeq L^{-1/2}$. Therefore

$$C = D \cos(kb + \delta)/\cosh \kappa b \simeq (2k/\kappa \sqrt{L}) e^{-\kappa b}, \tag{23}$$

by virtue of (20) and of $\kappa \gg k$, which follows from (6).

We are now ready to apply the golden rule, with $V = V_1$, defined by (4). We have

$$(\psi, V\phi) = -V_0 A C \int_{-a}^{a} \cos kx \cosh \kappa x \, dx. \tag{24}$$

The integral is readily evaluated† as $k \sin ka \, e^{\kappa a}/mV_0$ by using (17) and (18) and we finally obtain

$$\Gamma = 2\pi\rho(E_0)|(\psi, V\phi)|^2 = \pi^3 e^{-2\kappa(b-a)}/2m^2 a^4 V_0. \tag{25}$$

Note that although this result was obtained by a variant of perturbation theory, it cannot be expanded in positive powers of V_0. Such an expansion would of course violate (6) and (7).

As a check, we may also compute Γ by the Gamow (1928) complex energy method which essentially amounts to finding the poles of the scattering amplitude. We now take the complete Hamiltonian (3) and write the wavefunction as

$$\begin{aligned}
\psi &= A \cos kx, & x &\leq a, \\
&= B(e^{\kappa x} + Ce^{-\kappa x}), & a &\leq x \leq b, \\
&= D e^{ikx}, & x &\geq b.
\end{aligned} \tag{26}$$

We require ψ'/ψ to be continuous at $x = a$ and $x = b$, eliminate C from the two resulting equations and get

$$\frac{k}{\kappa} \tan ka = \frac{\kappa - ik - e^{-2\kappa(b-a)}(\kappa + ik)}{\kappa - ik + e^{-2\kappa(b-a)}(\kappa + ik)} \tag{27}$$

$$\simeq 1 - 2(1 + 2ik/\kappa) e^{-2\kappa(b-a)}, \tag{28}$$

the last step because $|\kappa|$ is large. However, the imaginary part of κ is very small, and it follows that

$$\text{Im}(\tan ka) \simeq -4 e^{-\kappa(b-a)} \tag{29}$$

or

$$\text{Im}(ka) \simeq -4 e^{-\kappa(b-a)}/(1 + \tan^2 ka) \simeq -4 e^{-\kappa(b-a)} k^2/\kappa^2, \tag{30}$$

by virtue of (18). Thus finally

$$\frac{\Gamma}{2} = -\text{Im}\left(\frac{k^2}{2m}\right) \simeq -\frac{k}{m} \text{Im}(k) \simeq \frac{\pi^3 e^{-\kappa(b-a)}}{4m^2 a^4 V_0}, \tag{31}$$

† This is an oversimplified argument. Actually, we could compute $(\psi, V\phi)$ by using an arbitrary E for ψ. In other words, k and κ in (19) need not be the same as k and κ in (18). However, if we are interested only in the final formula (25), we may immediately take E in $\psi(E)$ as the mean energy of state ϕ.

in agreement with (25). The same result was also obtained by Lubenets (1977) by directly integrating the time-dependent Schrödinger equation. See also Emch and Sinha (1979) for a different method.

Acknowledgments

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