XI. BACK TO THE TWO NEGATIVE DELTA FUNCTION PROBLEM

This all formal distraction really wanted to solve a simple question - what do the bound states of two negative delta functions at reasonably close proximity do.

Let us summarize what we know so far. In a potential well:

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V\delta(x) \tag{293}$$

there is a bound state,

$$|\psi\rangle = \sqrt{\kappa}e^{-\kappa|x|} \tag{294}$$

with $\kappa = mV/\hbar^2$ and energy:

$$E = -\frac{mV^2}{2\hbar^2}. \tag{295}$$

There are also a bunch of propagating states.

Now, consider the problem of having two of these delta-function wells in relatively close proximity:

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V(\delta(x-a) + \delta(x+a)). \tag{296}$$

How many bound states do you think there would be? It is reasonably easy to reason that there will be two - one for each well (this is true if the wells are not too close). But which two? If we think that the two states are simply:

$$|L\rangle \approx \sqrt{\kappa}e^{-\kappa|x+a|}, \quad |R\rangle \approx \sqrt{\kappa}e^{-\kappa|x-a|} \tag{297}$$

then we have to admit that we are wrong: the left bound state has a finite overlap with the potential well on the right - it may want to leak to it! Similarly, the bound state of the right well, $|R\rangle$ overlaps with the left well. What do you think would make sense? As a hint, think of the two lowest states of the particle in a box, and see if you can get inspiration from there.

Indeed, the lowest states should be the symmetric and antisymmetric superposition of the two states:

$$|+\rangle \approx \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle) \quad |-\rangle \approx \frac{1}{\sqrt{2}}(|R\rangle - |L\rangle) \tag{298}$$

why the approximation sign? Really because of the normalization. There is a finite overlap between the two wave-functions, and therefore the normalization is a bit different than $\sqrt{2}^{-1}$.

Eq. (298) is a pretty good guess for the two bound states. What are their energies? Initially they have the same energy - in the absence of the other delta function. But now there will be what we call - degeneracy breaking. What do you think its strength will be? exponential.

All we need to do is calculate the expectation value of the energy. This produces quite a few terms. As always, we can deal with all these terms by making some stories to go along with them. the energy expectation value is:

$$E_+ = \frac{\langle +|\hat{\mathcal{H}}|+\rangle}{\langle +|+\rangle} = \frac{1}{2}\frac{(\langle L| + \langle R|)\left(\hat{\mathcal{H}}|L\rangle + \hat{\mathcal{H}}|R\rangle\right)}{1 + |R\rangle\, L\rangle} \tag{299}$$

where we made use of the realness of the wavefunctions, and the fact that they are normalized albeit not orthogonal.

The idea now is to divide and conquer: apply the hamiltonian separately to the left and right bound state. Furhtermore:

$$numerator = \frac{1}{2}(\hat{\mathcal{H}}_{LL} + \hat{\mathcal{H}}_{RR} + \hat{\mathcal{H}}_{RL} + \hat{\mathcal{H}}_{LR}) \tag{300}$$

with $\hat{\mathcal{H}}_{AB} = \langle A|\, B\rangle$. This should remind you of something - it is the effective hamiltonian applied to the subspace of bound states. We can definitely think of this as:

$$\hat{\mathcal{H}}_{AB} = \begin{pmatrix} \hat{\mathcal{H}}_{LL} \approx E & \hat{\mathcal{H}}_{LR} \\ \hat{\mathcal{H}}_{RL} & \hat{\mathcal{H}}_{RR} \approx E \end{pmatrix} \tag{301}$$

diagonalizing it is indeed $(1,1)$ and $(1,-1)$. With Eigenvalues:

$$E_{\pm} = E \pm |\hat{\mathcal{H}}_{LR}|. \tag{302}$$

Let's now do the calculation. knowing that the left and right bound states:

$$\hat{\mathcal{H}}_{LL} = \langle L| - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V\delta(x-a)\,|L\rangle - V\,\langle L|\,\delta(x-a)\,|L\rangle \tag{303}$$

This is neat, because by writing things like this I isolated the part of the hamilotonian for which $|L\rangle$ is an exact ground state, and a delta function. The delta function contribution here is truly negligible - $e^{-4\kappa a}$. The result for the diagonal element is simply:

$$\hat{\mathcal{H}}_{LL} = -\frac{mV^2}{\hbar^2} - V\sqrt{\kappa}e^{-4\kappa L} \approx -\frac{1}{2\hbar^2}mV^2 \tag{304}$$

By symmetry:

$$\hat{\mathcal{H}}_{RR} = \hat{\mathcal{H}}_{LL} \approx -\frac{mV^2}{\hbar^2} \tag{305}$$

as well. and the mystery term is $\hat{\mathcal{H}}_{RL}$ which we can write as:

$$\hat{\mathcal{H}}_{RL} = \langle R| - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V\delta(x-a)\,|L\rangle - V\,\langle R|\,\delta(x-a)\,|L\rangle \tag{306}$$

Notice that I handled this hamiltonian in the same way, and operating on $|L\rangle$, we still get the $E\,|L\rangle$. This together gives:

$$\hat{\mathcal{H}}_{RL} = -\frac{mV^2}{2\hbar^2}\,\langle R|\,L\rangle - V\kappa e^{-2\kappa L}. \tag{307}$$

There is an overlap appearing here. This is not too threatening given that there is also a denominator. putting everything together we get:

$$E_{+} = -\frac{mV^2}{2\hbar^2}\frac{1+\langle R|\,L\rangle}{1+\langle R|\,L\rangle} - \frac{V\kappa e^{-2\kappa L}}{1+\langle R|\,L\rangle} \tag{308}$$

and if we trace back all the signs, and try to calculate the expectation of $E_{-} = \langle -|\,\hat{\mathcal{H}}\,|-\rangle\,/\,\langle -|\,-\rangle$ we get:

$$E_{\pm} \approx -\frac{mV^2}{2\hbar^2} \mp V\kappa e^{-2\kappa L} \tag{309}$$

neglecting pieces subleading in $e^{-2\kappa a}$.

We now can also look back and see how to interpret every term in the hamiltonian. The diagonal terms in the effective hamiltonian are nothing but the energy of each state. The off diagonal terms have a very simple meaning - the tunneling rate between the two wells.

A. Rabi oscillations

To appreciate that let us consider the time dependent SE. Bringing back the time dependence to the two-well bound states subspace, we have:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_L\\ \psi_R\end{pmatrix} = \begin{pmatrix}\hat{\mathcal{H}}_{LL} & \hat{\mathcal{H}}_{RL}\\ \hat{\mathcal{H}}_{RL} & \hat{\mathcal{H}}_{RR}\end{pmatrix}\begin{pmatrix}\psi_L\\ \psi_R\end{pmatrix} \tag{310}$$

and this we approximate as:

$$= \begin{pmatrix}E_0 & -J\\ -J & E_0\end{pmatrix}\begin{pmatrix}\psi_L\\ \psi_R\end{pmatrix} \tag{311}$$

And we already have the eigenstates of this Hamiltonian above. Now, suppose we put a particle in the left well (or measure a particle to be in the left well), how does it evolve?

The first thing to appreciate is that we can still use sparation of variables to solve the time-dependent matrix Schrdinger equation, eq. (310). The entries ψ_L and ψ_R are essentially like the wave functions at the right well and the left well, so they constitute a simplification of $\psi(x)$. Separation of variables would then imply looking for solutions in the form:

$$\begin{pmatrix} \psi_L(t) \\ \psi_R(t) \end{pmatrix} = f(t) \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}. \tag{312}$$

Plugging this in we see that Eq. (310) becomes:

$$i\hbar \frac{1}{f}\frac{\partial f}{\partial t} \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = \begin{pmatrix} E_0 & -J \\ -J & E_0 \end{pmatrix} \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}. \tag{313}$$

For the RHS of this equation to be time indepedent we require:

$$i\hbar \frac{1}{f}\frac{\partial f}{\partial t} = E \tag{314}$$

with E being a constant. Indeed, this should look familiar - E is just the new energy. But if this is so, we end up with

$$f(t) = e^{-iEt/\hbar} \tag{315}$$

and (ψ_L, ψ_R) must be an eigenvector of H_{AB} in Eq. (301), with E being the eigenvalue.

Once we obtain the two eigenvalues and eigenvectors, $|+\rangle$ with energy E_+ and $|-\rangle$ with energy E_-, we can construct the general time-dependent solution:

$$|\psi(t)\rangle = \alpha\, |+\rangle\, e^{-iE_+t/\hbar} + \beta\, |-\rangle\, e^{-iE_-t/\hbar}. \tag{316}$$

α and β need to be chosen according to the initial conditions.

Let us solve for the time evolution of a particle that finds itself squarely in the left well at $t = 0$. In this case, the wave function strats off simply: $\psi_L = 1$, $\psi_R = 0$. This we can write using the symmetric and antisymmetric combinations, which are the eigenstates of the problem:

$$|\psi(t=0)\rangle = |L\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle + |-\rangle\right) \tag{317}$$

adding the time dependence we get, using $E_\pm = E_0 \mp J$:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle\, e^{-i(E-J)t/\hbar} + |-\rangle\, e^{-i(E+J)t/\hbar}\right). \tag{318}$$

To make sense out of this we should revert to a description in terms of the original kets, $|L\rangle$, $|R\rangle$, which gives:

$$|\psi(t)\rangle = e^{-iE_0t/\hbar} \left(|L\rangle \cos(Jt/\hbar) + i\, |R\rangle \sin(Jt/\hbar)\right) \tag{319}$$

The particle seems to be moving back and forth between the two wells. This motion is called Rabi oscillations. The Rabi angular frequency is indeed $\frac{J}{\hbar}$. Note that the probability with which the particles oscillate from side to side is $J/\hbar\pi$; the probabilities of the particle being in the left (initial) and right wells are:

$$p_L = |\,\langle L|\, |\psi(t)\rangle\,|^2 = \cos^2(Jt/\hbar), \;\; p_R = |\,\langle R|\, |\psi(t)\rangle\,|^2 = \sin^2(Jt/\hbar). \tag{320}$$