VARIATIONAL PRINCIPLE WITH A TWO-STATE HAMILTONIAN

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.15.

Suppose we have a system with just two possible energies and corresponding eigenstates, which we'll call ψ_a with energy E_a and ψ_b with energy E_b, with $\langle a|b\rangle = 0$, $\langle a|a\rangle = \langle b|b\rangle = 1$ $E_a < E_b$. Now we turn on a perturbation H' which has the matrix elements

$$H' = \begin{bmatrix} 0 & h \\ h & 0 \end{bmatrix} \tag{1}$$

The total hamiltonian is now $H = H_0 + H'$, where H_0 is the unperturbed hamiltonian. The matrix elements of H are then

$$H = \begin{bmatrix} E_a & h \\ h & E_b \end{bmatrix} \tag{2}$$

so the exact perturbed energies are the eigenvalues of this matrix, which are

$$E' = \frac{1}{2}\left(E_a + E_b \pm \sqrt{(E_a - E_b)^2 + 4h^2}\right) \tag{3}$$

Now we can apply perturbation theory to this problem. Since the diagonal matrix elements of H' are both zero, the first order perturbation is also zero. The second order perturbation is

$$E_{n2} = \sum_{j\neq n} \frac{|\langle j0|H'|n0\rangle|^2}{E_{n0} - E_{j0}} \tag{4}$$

This gives for the perturbations on the two energies:

$$E_{a2} = \frac{h^2}{E_a - E_b} \tag{5}$$

$$E_{b2} = \frac{h^2}{E_b - E_a} \tag{6}$$

If we expand 3 in a Taylor series, these are second order terms in the series.

Finally, we can use the variational principle with the trial function

$$\psi=(\cos\phi)\,\psi_a+(\sin\phi)\,\psi_b=\left[\begin{array}{c}\cos\phi\\ \sin\phi\end{array}\right] \tag{7}$$

We can calculate $\langle H\rangle$ as follows:

$$\begin{aligned}
\langle H\rangle &= \psi^T H\psi && (8)\\
&= \left[\begin{array}{cc}\cos\phi & \sin\phi\end{array}\right]\left[\begin{array}{cc}E_a & h\\ h & E_b\end{array}\right]\left[\begin{array}{c}\cos\phi\\ \sin\phi\end{array}\right] && (9)\\
&= E_a\cos^2\phi+E_b\sin^2\phi+2h\sin\phi\cos\phi && (10)
\end{aligned}$$

The variable parameter here is ϕ so we take the derivative with respect to it and set to zero to get the minimum energy:

$$\begin{aligned}
\frac{d\langle H\rangle}{d\phi} &= (E_b-E_a)(2\sin\phi\cos\phi)+2h\left(\cos^2\phi-\sin^2\phi\right) && (11)\\
&= (E_b-E_a)\sin2\phi+2h\cos2\phi=0 && (12)\\
\tan2\phi_{min} &= -\frac{2h}{E_b-E_a} && (13)\\
\sin2\phi_{min} &= -\frac{2h}{E_b-E_a}\cos2\phi_{min} && (14)\\
\cos2\phi_{min} &= \frac{1}{\sqrt{1+\tan^2 2\phi_{min}}} && (15)\\
&= \left(1+\frac{4h^2}{(E_b-E_a)^2}\right)^{-1/2} && (16)\\
&= \frac{E_b-E_a}{\sqrt{(E_b-E_a)^2+4h^2}} && (17)
\end{aligned}$$

We can express $\langle H\rangle_{min}$ using trig identities:

$$\begin{aligned}
\langle H\rangle_{min} &= \frac{1}{2}(1+\cos2\phi_{min})E_a+\frac{1}{2}(1-\cos2\phi_{min})E_b+h\sin2\phi_{min} && (18)\\
&= \frac{1}{2}\left(E_a+E_b-\sqrt{(E_a-E_b)^2+4h^2}\right) && (19)
\end{aligned}$$

which is exactly the lower of the two exact energies 3. The variational principle gives the exact answer because the trial function is the exact eigenfunction, with ϕ_{min} giving the components of the two unperturbed eigenfunctions that make up the perturbed eigenfunction.

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