11.3: Two-State System

Consider the simplest possible non-trivial quantum mechanical system. In such a system, there are only two independent eigenstates of the unperturbed Hamiltonian: that is,

$$\begin{aligned} H_0\,\psi_1 &= E_1\,\psi_1,\\ H_0\,\psi_2 &= E_2\,\psi_2. \end{aligned}$$

It is assumed that these states, and their associated eigenvalues, are known. We also expect the states to be orthonormal, and to form a complete set.

Let us now try to solve the modified energy eigenvalue problem

$$(H_0+H_1)\,\psi_E = E\,\psi_E. \tag{11.3.1}$$

We can, in fact, solve this problem exactly. Because the eigenstates of H_0 form a complete set, we can write [see Equation ([e12.13a])]

$$\psi_E = \langle 1|E\rangle\,\psi_1 + \langle 2|E\rangle\,\psi_2. \tag{11.3.2}$$

It follows from Equation ([e12.23]) that

$$\langle i|H_0+H_1|E\rangle = E\,\langle i|E\rangle, \tag{11.3.3}$$

where $i=1$ or 2. Equations ([e12.21]), ([e12.22]), ([e12.24]), ([e12.25]), and the orthonormality condition

$$\langle i|j\rangle = \delta_{ij}, \tag{11.3.4}$$

yield two coupled equations that can be written in matrix form:

$$\begin{pmatrix} E_1-E+e_{11}, & e_{12}\\ e_{12}^\ast, & E_2-E+e_{22}\end{pmatrix}\begin{pmatrix}\langle 1|E\rangle\\ \langle 2|E\rangle\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix},$$

where

$$\begin{aligned} e_{11} &= \langle 1|H_1|1\rangle,\\ e_{22} &= \langle 2|H_1|2\rangle,\\ e_{12} &= \langle 1|H_1|2\rangle = \langle 2|H_1|1\rangle^\ast. \end{aligned}$$

Here, use has been made of the fact that H_1 is an Hermitian operator.

Consider the special (but not uncommon) case of a perturbing Hamiltonian whose diagonal matrix elements are zero, so that

$$e_{11}=e_{22}=0. \tag{11.3.5}$$

The solution of Equation ([e12.27]) (obtained by setting the determinant of the matrix to zero) is

$$E = \frac{(E_1+E_2)\pm\sqrt{(E_1-E_2)^{\,2}+4\,|e_{12}|^{\,2}}}{2}. \tag{11.3.6}$$

Let us expand in the supposedly small parameter

$$\epsilon = \frac{|e_{12}|}{|E_1-E_2|}. \tag{11.3.7}$$

We obtain

$$E \simeq \frac{1}{2}\,(E_1+E_2)\pm\frac{1}{2}\,(E_1-E_2)(1+2\,\epsilon^{\,2}+\cdots). \tag{11.3.8}$$

The previous expression yields the modification of the energy eigenvalues due to the perturbing Hamiltonian:

$$E_1' = E_1 + \frac{|e_{12}|^2}{E_1 - E_2} + \cdots,$$
$$E_2' = E_2 - \frac{|e_{12}|^2}{E_1 - E_2} + \cdots.$$

Note that H_1 causes the upper eigenvalue to rise, and the lower to fall. It is easily demonstrated that the modified eigenstates take the form

$$\psi_1' = \psi_1 + \frac{e_{12}^*}{E_1 - E_2}\,\psi_2 + \cdots,$$
$$\psi_2' = \psi_2 - \frac{e_{12}}{E_1 - E_2}\,\psi_1 + \cdots.$$

Thus, the modified energy eigenstates consist of one of the unperturbed eigenstates, plus a slight admixture of the other. Now, our expansion procedure is only valid when $\epsilon \ll 1$. This suggests that the condition for the validity of the perturbation method as a whole is

$$|e_{12}| \ll |E_1 - E_2|. \tag{11.3.9}$$

In other words, when we say that H_1 needs to be small compared to H_0, what we are really saying is that the previous inequality must be satisfied.

Contributors and Attributions

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