

Nearly every problem we have solved thus far has had an exact solution. However most systems require that we solve them approximately b/c typically they are too complex to yield exact analytical solutions. (5)

The role of Perturbation Theory is to offer a framework for some class of these problems where the Hamiltonian can be separated into a part we can solve exactly and a part we believe has a small effect so that our solution can be approximated (typically analytically but not exclusively so).

We will introduce the general problem for a two state system and then

Show a specific example for Spin $1/2$.

General Two Level Problem

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For a general Two Level Problem our Hilbert space is 2D. We can formalize this by considering the energy eigenstates for the "original" or zeroth order Hamiltonian,

$$H = H_0 + H' \leftarrow \begin{array}{l} \text{perturbation} \\ \text{Hamiltonian,} \end{array}$$

\uparrow original / zeroth order

zeroth order

$$H_0 = \begin{pmatrix} E_1^{(0)} & 0 \\ 0 & E_2^{(0)} \end{pmatrix}$$

$$H_0 |1\rangle = E_1^{(0)} |1\rangle$$

$$H_0 |2\rangle = E_2^{(0)} |2\rangle$$

perturbation

In the basis of the original Hamiltonian we consider a general perturbation,

$$H' = \begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix}$$

It is common to introduce a parameter λ (3) that we later set to 1 to keep track of the order of corrections

$$\left(\begin{array}{l} \lambda \rightarrow \text{first order} \\ \lambda^2 \rightarrow \text{second order} \\ \text{etc.} \end{array} \right)$$

$$H = H_0 + \lambda H' = \begin{pmatrix} E_1^{(0)} + \lambda H'_{11} & \lambda H'_{12} \\ \lambda H'_{21} & E_2^{(0)} + \lambda H'_{22} \end{pmatrix}$$

Note $H'_{12} = H'_{21}^\dagger \Rightarrow H$ must be Hermitian

$H = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}$ is the form of H

Can we find the exact eigenvalues?

$$H - IE = \begin{pmatrix} a - E & c \\ c^* & b - E \end{pmatrix}$$

$$\det(H - IE) = 0 \iff$$

$$(a - E)(b - E) - cc^* = 0$$

$$E^2 - E(a+b) + ab - |c|^2 = 0$$

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Quadratic Eqn.

$$E = \frac{a+b \pm \sqrt{(a+b)^2 - 4(ab - |c|^2)}}{2}$$

$$= \frac{1}{2}(a+b) \pm \sqrt{\frac{1}{4}(a+b)^2 - ab + |c|^2}$$

$$E = \frac{1}{2}(a+b) \pm \sqrt{\frac{1}{4}(a-b)^2 + |c|^2} \quad \text{Exact Solution}$$

But we assume the contributions of H' are much smaller than H_0 ,

so that $(b-a) \gg c$

Approximate Solutions?

$$E = \frac{1}{2}(a+b) \pm \frac{1}{2}(a-b) \left[1 + \frac{4|c|^2}{(a-b)^2} \right]^{1/2}$$

$$E \approx \frac{1}{2}(a+b) \pm \frac{1}{2}(a-b) \left[1 + \frac{2|c|^2}{(a-b)^2} \right] \quad \text{Approx Solutions}$$

$$E_1 \approx \frac{1}{2}(a+b) + \frac{1}{2}(a-b) \left[1 + \frac{2|c|^2}{(a-b)^2} \right]$$

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$$E_1 \approx a + \frac{|c|^2}{(a-b)}$$

$$E_2 \approx \frac{1}{2}(a+b) - \frac{1}{2}(a-b) \left[1 + \frac{2|c|^2}{(a-b)^2} \right]$$

$$E_2 \approx b - \frac{|c|^2}{(a-b)}$$

Recall $a = E_1^{(0)} + \lambda H'_{11}$ $b = E_2^{(0)} + \lambda H'_{22}$
 $c = \lambda H'_{12}$ $c^* = \lambda H'_{21}$

Translate this back to H_0 & H' ,

$$E_1 \approx E_1^{(0)} + \lambda H'_{11} + \frac{\lambda^2 |H'_{12}|^2}{(E_1^{(0)} + \lambda H'_{11} - E_2^{(0)} - \lambda H'_{22})}$$

$$E_2 \approx E_2^{(0)} + \lambda H'_{22} + \frac{\lambda^2 |H'_{21}|^2}{(E_1^{(0)} + \lambda H'_{11} - E_2^{(0)} - \lambda H'_{22})}$$

To second order in λ ,

$$E_1 \approx E_1^{(0)} + \lambda H'_{11} + \lambda^2 \frac{|H'_{12}|^2}{(E_1^{(0)} - E_2^{(0)})}$$

$$E_2 \approx E_2^{(0)} + \lambda H'_{22} + \lambda^2 \frac{|H'_{21}|^2}{(E_2^{(0)} - E_1^{(0)})}$$

We set $\lambda=1$ and we can keep track of each contribution with $E_i^{(n)}$ where i is the state and (n) represents the correction order,

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$$E_i \approx E_i^{(0)} + E_i^{(1)} + E_i^{(2)}$$

Two State System

$E_i^{(0)} \Rightarrow$ unperturbed energy, H_{ii}

$E_i^{(1)} \Rightarrow$ first order correction, H'_{ii}

$E_i^{(2)} \Rightarrow$ second order correction, $\frac{|H_{ij}|^2}{(E_i^{(0)} - E_j^{(0)})}$