perturbation theory

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recapitulation: perturbation theory

Assuming we know eigenvalues and eigenfunctions of a hamiltonian H_0:

$$H_0\,|\,n_0> = E_n^0\,|\,n_0>$$

what are the eigenvalues and eigenfunctions of a hamiltonian H that has the form

$$H \;=\; H_0 + \epsilon\, H_1 + \epsilon^2\, H_2 + \ldots$$

where ε is a small number (<< 1) ?

(Note: H_2 can be zero).

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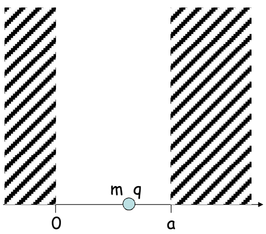
Example 1: charged particle in an infinitely deep potential well



$$\hat{H}_0 \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$E_{0,N} \;=\; \frac{\hbar^2\pi^2}{2ma^2}N^2 \qquad (N \;=\; 1,2,3,\ldots)$$

$$\Psi_{0,N}(x) \;=\; \sqrt{\frac{2}{a}}\,\sin\frac{N\pi x}{a}$$

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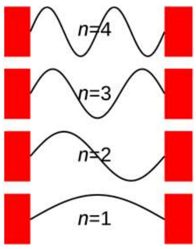

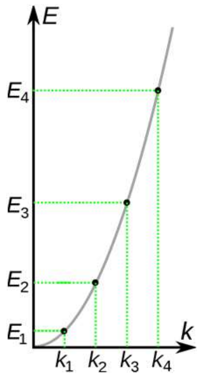

(pictures taken from Wikipedia)

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perturbation: constant electric field

electric field : $\vec{E}(x) = K\vec{e}_x$

potential energy: $V(x) = -qKx$

perturbing operator: $\hat{H}_1 = -qK\hat{x}$

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - qKx$$

form of hamiltonian $\propto \frac{d^2}{dx^2} + \underbrace{\frac{2qmK}{\hbar^2}}_{\text{small if the electric field is not too strong}} x$

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Solution up to first order in ε :

1) non-degenerate case

For eigenvalues that are non-degenerate (i.e. H_1 does not lift any degeneracy), the new eigenvalues and eigenfunctions are given by:

$$\Delta E_n^1 = <n_0| \; H_1 | n_0>$$

$$\Rightarrow \quad E_{\tilde{n}} = E_n^0 + \epsilon \Delta E_n^1$$

$$|\tilde{n}_1> = \sum_{m \neq n} \frac{<m_0| \; H_1 | n_0>}{E_n^0 - E_m^0} | m_0>$$

$$\Rightarrow \quad |\tilde{n}> = |n_0> + \epsilon |n_1>$$

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Application to example 1:

$$\Delta E_N^1 = \langle \Psi_{0,N} | \hat{H}_1 | \Psi_{0,N} \rangle$$
$$= -\frac{2qK}{a} \int x \sin^2 \frac{N\pi x}{a} \, dx$$
$$= -\frac{qKa}{2}$$

Downward shift of all levels, independent of N.

Exercise: find the wave functions and probability density.

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Solution up to first order in ε :

2) l-fold degenerate case

For eigenvalues that are degenerate (i.e. H_1 does lift a degeneracy), the new eigenvalues and eigenfunctions are found by this procedure:

➔ orthonormalize
Find an orthonormal basis $| n_0^i >$ for the l-dimensional subspace

➔ diagonalize
The l energy corrections are found as the l eigenvalues of this matrix:

$$\begin{bmatrix} <n_0^1| \epsilon H_1 | n_0^1> & <n_0^1| \epsilon H_1 | n_0^2> & \cdots & <n_0^1| \epsilon H_1 | n_0^\ell> \\ <n_0^2| \epsilon H_1 | n_0^1> & <n_0^2| \epsilon H_1 | n_0^2> & \cdots & <n_0^2| \epsilon H_1 | n_0^\ell> \\ \vdots & \vdots & \ddots & \vdots \\ <n_0^\ell| \epsilon H_1 | n_0^1> & <n_0^\ell| \epsilon H_1 | n_0^2> & \cdots & <n_0^\ell| \epsilon H_1 | n_0^\ell> \end{bmatrix}$$

The new eigenstates are the eigenvectors of this matrix.

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Example 2: free electron under an applied magnetic field

without field, up and down spin are degenerate: $\Psi_\uparrow \quad \Psi_\downarrow$

$$\hat{H}_0 = \hat{1\!\!1}$$
$$\hat{H}_1 = -\hat{\vec{\mu}} \cdot \vec{B}$$
$$= -\left(\frac{-2\mu_B \hat{\vec{S}}}{\hbar} \right) \cdot \vec{B}$$

$$\begin{bmatrix} \langle \Psi_\uparrow | \hat{S}_z | \Psi_\uparrow \rangle & \langle \Psi_\uparrow | \hat{S}_z | \Psi_\downarrow \rangle \\ \langle \Psi_\downarrow | \hat{S}_z | \Psi_\uparrow \rangle & \langle \Psi_\downarrow | \hat{S}_z | \Psi_\downarrow \rangle \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\hbar & 0 \\ 0 & -\frac{1}{2}\hbar \end{bmatrix}$$

This is already diagonal.

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A derivation and more examples can be found at

http://en.wikipedia.org/wiki/Perturbation_theory_(quantum_mechanics)

(section 2.1, 2.2 and 5)

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