PERTURBATION THEORY

Assume H can be written as

$$H = H_0 + \lambda V \qquad (1)$$

where λ is a <u>parameter</u> that is adjustable, for example an external electric field. Also, assume we <u>know</u> the eigenfunctions and eigenvalues of H_0. Thus,

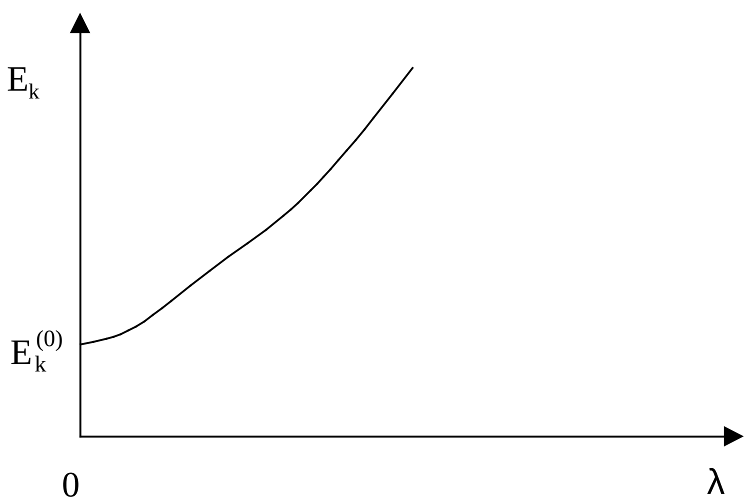
$$H_0 \varphi_k^{(0)} = E_k^{(0)} \varphi_k^{(0)} \qquad (2)$$

$\varphi_k^{(0}$ are termed the zero-order eigenfunctions;

$E_k^{(0)}$ are termed the zero-order eigenvalues.

We want eigs of H, i.e.,

$$H\psi_k = E_k \psi_k$$



$E_k(\psi)$ is assumed to be a “well-behaved” function. Thus,

$$E_k(\lambda) = E_k(\lambda = 0) + E_k'(0)\lambda + E_k''(0)\frac{\lambda^2}{2} + \ldots = E_k^{(0)} + E_k^{(1)}\lambda + E_k^{(2)}\lambda^2 + \ldots$$

Similarly,

$$\psi_k(\lambda) = \psi_k(\lambda = 0) + \psi_k'(0)\lambda + \psi_k''(0)\frac{\lambda^2}{2} + \ldots = \varphi_k^{(0)} + \varphi_k^{(1)} + \varphi_k^{(2)}\lambda^2 + \ldots$$

$E^{(1)}$ and $E^{(2)}$ are the first-order and second-order corrections to the energy, respectively. Similarly, $\varphi_k^{(1)}$ and $\varphi_k^{(2)}$ are first-order and second-order corrections to the wavefunction, respectively. See appendix D for the systematic derivations of the following results:

$$E_k^{(1)} = \int \varphi_k^{(0)} V \varphi_k^{(0)} d\tau = \langle \varphi_k^{(0)} | V | \varphi_k^{(0)} \rangle \tag{3}$$

$$E_k^{(2)} = \sum_{\ell \neq k} \frac{\left| \langle \varphi_k^{(0)} | V | \varphi_\ell^{(0)} \rangle \right|^2}{E_k^{(0)} - E_\ell^{(0)}} \tag{4}$$

$$\varphi_k^{(1)} = \sum_{\ell \neq k} \frac{\langle \varphi_\ell^{(0)} | V | \varphi_k^{(0)} \rangle}{E_k^{(0)} - E_\ell^{(0)}} \varphi_\ell^{(0)} \tag{5}$$

Example 1 (quartic oscillator)

$$H = H_{HO}(x) + \lambda x^4$$

$$E_n^{(1)} = \langle \varphi_n^{(0)} | x^4 | \varphi_n^{(0)} \rangle$$

$$E_n \approx E_n^{(0)} + \lambda \langle \varphi_n^{(0)} | x^4 | \varphi_n^{(0)} \rangle$$

--need to be able to do the integral. This one can be done analytically.