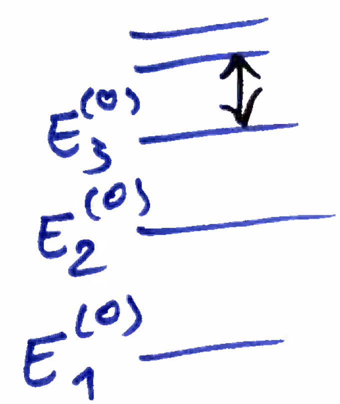
Bound perturbation formalism

(Summing up)

- Validity of the expansion depends on $|V_{nk}| / (E_n^{(0)} - E_k^{(0)}) \ll 1$



- Upto second order there is no tendency for the levels beginning to mix
  - g.s. $(n=1)$ is lowered in energy by second order correction

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Normalization

Suppose we calculate upto order N in pert. th. It is expedient to normalize the wavefunctions so obtained

$${}_N\langle n | n \rangle_N = 1$$ Assume the relation

nth level to order N

$$|n\rangle_N = Z_N^{1/2} |n\rangle_\lambda$$

and it means $\langle n^{(0)} | n \rangle_N = Z_N^{1/2}$

$$1 = Z_N \, {}_\lambda\langle n | n \rangle_\lambda = Z_N \left(1 + \lambda^2 \langle n^{(1)} | n^{(1)} \rangle + \cdots \right)$$

$$Z_N \simeq \left(1 + \lambda^2 \langle n^{(1)} | n^{(1)} \rangle \ldots\right)^{-1}$$

$$\langle n^{(1)} | n^{(1)} \rangle = \sum_k{}' \frac{|V_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2}$$

$$Z_N \simeq 1 - \lambda^2 \sum{}' \frac{|V_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2}$$

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Case of <u>degenerate</u> unperturbed states

("Degenerate pert. th.")

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Answers w/o proof : (proof in Merzbacher, Sakurai ...)

1 If a level is degenerate with eigenvectors $\{|l^{(0)}\rangle\} \equiv D$

Calculate the matrix $\langle l_i^{(0)} | V | l_j^{(0)} \rangle \equiv \mathbb{V}_{ij}$

Diagonalise matrix $\mathbb{V}$

The eigenvalues give splitting of the D space

2. For corrections to the eigenvectors we use formulae similar to those for non-deg. case, but with

$$\sum{}' \equiv \sum_{k \neq n} \xrightarrow{\text{replaced}} \sum_{k \notin D} \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} \ldots$$

for corrections to level n

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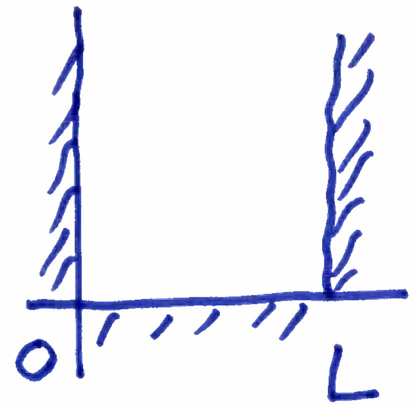
Example:

"Particle in a box" as H_0



perturbation

$$\alpha V = \alpha\,\delta(x - L/2)$$

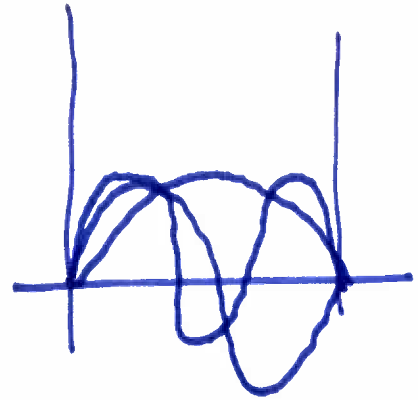
Recall

$$\psi_n^{(0)} = \sqrt{\frac{2}{L}}\,\sin\frac{n\pi}{L}x \qquad n = 1, 2, \ldots$$

$$E_n^{(0)} = \text{"}\frac{p_n^2}{2m}\text{"} = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$E_n^{(1)} = \langle n^{(0)}|\alpha V|n^{(0)}\rangle = \frac{2}{L}\alpha\int_0^L \delta(x - L/2)\,\overset{\sin^2}{\cancel{\cos^2}}\frac{n\pi}{L}x$$

$$\therefore \quad E_n^{(1)} = \begin{cases} \frac{2}{L}\alpha & n = 1, 3, \ldots \\ 0 & n = 2, 4, \ldots \end{cases}$$



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Consider $n = 1$ (g.s.)

$$V_{nk} \equiv V_{1k} = \alpha \frac{2}{L} \int_0^L \sin \frac{\pi}{L} x \cdot \sin \frac{k\pi}{L} x \, x \, dx$$

$$E_1^{(2)} = \sum_{k \neq 1} \frac{|V_{k1}|^2}{E_1 - E_k} = \sum_{r=1}^{\infty} \frac{2mL^2/\pi^2}{1 - (2r+1)^2}$$