S-Pset-2
MZ7 αW
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3. Developing the variational Principle

a) Trial $\psi(x)$ orthog^n to ψ_1 : $\int dx\, \psi_1(x)\psi(x)\, dx = 0$

Let $\psi(x) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$, $c_1 = 0$

Normalis^n $\Rightarrow \sum_n |c_n|^2 = 1$, $c_1 = 0 \Rightarrow \sum_{n=2}^{\infty} |c_n|^2$

$\int dx\, \psi^*(x) H \psi(x) = \langle H \rangle = \sum_n |c_n|^2 E_n$

now $c_1 = 0 \Rightarrow \langle H \rangle = \sum_{n=2}^{\infty} |c_n|^2 E_n$

$E_n > E_2 \;\; \forall n > 2 \Rightarrow \sum_{n=2}^{\infty} |c_n|^2 E_n > \sum_{n=2}^{\infty} |c_n|^2 E_2 > E_2 \cdot 1$

$\Rightarrow E_2 \leq \int dx\, \psi^*(x) H \psi(x)$

b) $F[\psi] = \dfrac{\int dx\, \psi^* \hat{H} \psi}{\int dx\, \psi^* \psi}$

let $\psi = \psi_2 + \sum_{n=1} \varepsilon_n \psi_n$,

$$F[\psi] = \frac{\int dx\, (\psi_2 + \sum_{n=1} \varepsilon_n \psi_n)^* \hat{H} (\psi_2 + \sum_{n=1} \varepsilon_n \psi_n)}{\int (\psi_2 + \sum_{n=1} \varepsilon_n \psi_n)^* (\psi_2 + \sum_{n=1} \varepsilon_n \psi_n)\, dx}$$

$$= \frac{E_2 + \sum_{n=1} |\varepsilon_n|^2 E_n + 2\varepsilon_2 E_2}{1 + \sum_{n=1} |\varepsilon_n|^2 + 2\varepsilon_2}$$ ($n=2$ has $(1+\varepsilon_2)E_2$ as expectation of $\hat{H}$)

This follows from orthogonality of ψ family

The question is ambiguous on whether $\varepsilon_2 = 0$ or not but I take it non-zero so that the perturbation is under no constraint

$$\Rightarrow \delta F[\psi] = \frac{\sum |\epsilon_n|^2 E_n + (1+2\varepsilon_2)E_2}{\sum |\epsilon_n|^2 + (1+2\varepsilon_2)}$$

$$\approx \left(\sum |\epsilon_n|^2 E_n + (1+2\varepsilon_2)E_2\right)\left(1 - 2\varepsilon_2 - \sum |\epsilon_n|^2\right)$$

or

$$\approx \left(\sum |\epsilon_n|^2 E_n + (1+2\varepsilon_2)E_2\right)\left(1 - 2\varepsilon_2 - \sum |\epsilon_n|^2 + (2\varepsilon + \sum |\epsilon_n|^2)^2\right)$$

~~for~~ Zoroth order: E_2

First order: $2\varepsilon_2 E_2 - 2\varepsilon_2 E_2 = 0$

Second order: $\sum |\varepsilon_n|^2 (E_n - E_2) - 4\varepsilon_2^2 E_2 + 4\varepsilon_2^2 E_2$

$$= \sum |\varepsilon_n|^2 (E_n - E_2)$$

$\Rightarrow$ ε_2 drops out to quadratic order

since in $\sum |\varepsilon_n|^2 (E_n - E_2)$, $|\varepsilon_2|^2$ will have $E_2 - E_2 = 0$ slopped

Note $|\varepsilon_1|^2$ has $(E_1 - E_2)$ multiplied

$\Rightarrow \delta F = F[\psi] - F[\psi_2] = \sum |\varepsilon_n|^2 (E_n - E_2) + O(\varepsilon^3)$

then $\forall\ \psi_i\ ;\ i > 2,\ \frac{\delta F}{\varepsilon_i} > 0,$ for $\psi_1\ \frac{\partial F}{\partial \varepsilon_1} < 0$

$\Rightarrow F[\psi_2]$ is a ~~static~~ saddle point.

If we view it in energy eigenbasis,

the point $(0, 1, 0, 0, \ldots)$ is a saddle point

since moving along $(\varepsilon, 0, 0, 0, \ldots)$ $\downarrow F[\psi_2]$ in 2^{nd} order

$(0, 0, 0, \ldots, \varepsilon_i, \ldots)$ will $\uparrow F[\psi_2]$ in 2^{nd} order

while motion along $(0, \varepsilon_2, 0, 0, \ldots)$ will have no effect or flat direc^n it is.

(So for $F[\psi_1]$, any motion $\uparrow F[\psi]$, thus the variational principle and this explains why in a), $c_1 = 0$)