6.878 Lecture

10/16/19

From last time: Variational Method

Trial Wavefunction: $\psi_t[\alpha, \beta \ldots]$

Total energy $\epsilon_t[\alpha, \beta \ldots] = \dfrac{\langle \psi_t[\alpha,\beta \ldots] | \hat{H} | \psi_t[\alpha, \beta \ldots] \rangle}{\langle \psi_t[\alpha, \beta \ldots] | \psi_t[\alpha, \beta, \ldots] \rangle}$

$\dfrac{\partial}{\partial \alpha} \epsilon_t = 0$

$\dfrac{\partial}{\partial \beta} \epsilon_t = 0$ $\Rightarrow \epsilon_t[\alpha_{opt}, \beta_{opt} \ldots]$

est. method for (8 highest eigenvalues

Why it works

$\psi_t = \sum_j a_j \phi_j \Rightarrow \epsilon_t = \dfrac{\sum_j |a_j|^2 E_j}{\sum_j |a_j|^2}$ $\quad E_j \phi_j = \hat{H} \phi_j$

$\epsilon_{opt} = 3.84748$

$\epsilon \psi = -\dfrac{d^2}{dy^2}\psi(y) + y^4 \psi(y)$

$\epsilon_{exact} = 3.7997\ldots$

$\psi_t(y) = \left(\dfrac{32\alpha^3}{\pi}\right)^{1/4} y\, e^{-\alpha y^2}$ $\quad \epsilon_t = \langle \psi_t | -\dfrac{d^2}{dy^2} + y^4 | \psi_t \rangle$

$= 3\alpha + \dfrac{15}{16\alpha^2}$

$\dfrac{\partial}{\partial \alpha} \epsilon_t = 0 \Rightarrow \alpha_{opt} = \frac{9}{4} \beta^{1/3}$

→ Finite basis approximation

→ 2 level systems

- Extract 2-level $\hat{H}$ (approx $\hat{H}$)
- State problem, $\sum_j a_j \phi_j e^{iE_j t/\hbar}$, Rabi oscillations

pset: Rotation → basis transformation - perturbation

dynamic model, Ehrenfest's theorem, block eq'ns & laser eq'ns

coupled systems → two-level system coupled in harmonic oscillator

SHO + 2 level system.

Finite basis approximation

$\psi_t[c_1, c_2] = \sum_j c_j u_j(x) = c_1 u_1(x) + c_2 u_2(x)$

$\langle u_1 | u_2 \rangle = 0$

$\langle u_1 | u_1 \rangle = \langle u_2 | u_2 \rangle = 1$

$E_t[c_1, c_2] = \dfrac{\langle \psi_t | \hat{H} | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} = \dfrac{\langle c_1 u_1 + c_2 u_2 | \hat{H} | c_1 u_1 + c_2 u_2 \rangle}{\langle c_1 u_1 + c_2 u_2 | c_1 u_1 + c_2 u_2 \rangle}$

$= \dfrac{c_1^2 \langle u_1 | \hat{H} | u_1 \rangle + c_1 c_2 \langle u_1 | \hat{H} | u_2 \rangle + c_2 c_1 \langle u_2 | \hat{H} | u_1 \rangle + c_2^2 \langle u_2 | \hat{H} | u_2 \rangle}{c_1^2 + c_2^2}$

$H_{jK} = \langle u_j | \hat{H} | u_K \rangle$

$O_{jK} = \langle u_j | u_K \rangle$

$$E_t = \frac{C_1^2 H_1 + 2C_1C_2H_{12} + C_2^2 H_{22}}{C_1^2 + C_2^2}$$

$$\frac{\partial}{\partial C_1} E_t = \frac{2C_1 H_{11} + 2C_2 H_{12}}{C_1^2 + C_2^2}$$

$$-(2C_1)\frac{C_1^2 H_{11} + 2C_1C_2H_{12} + C_2^2 H_{22}}{(C_1^2 + C_2^2)^2}$$

$$H_{11} C_1 + H_{12} C_2 = \frac{C_1^2 H_{11} + 2C_1C_2H_{12} + C_2^2 H_{22}}{C_1^2 + C_2^2} C_1$$

$$\frac{\partial}{\partial C_2} E_t[C_1, C_2] = 0 \Longrightarrow H_{21} C_1 + H_{22} C_2 = E_t C_2$$

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = E_t \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} \qquad \vec{H} \cdot \vec{C} = E_t \vec{C}$$

$$\psi_t = \sum_{j=1}^{N} C_j u_j$$

Finite basis constituents most widely used !!!

$$\epsilon \psi(y) = -\frac{d^2}{dy^2}\psi(y) + y^4 \psi(y)$$

Harmonic oscillator $\longleftrightarrow$ Quartic well... similarity?

$$u_1(y) = \frac{1}{\pi^{1/4}} e^{-y^2/2} = \phi_0(y)$$

$$u_2(y) = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2}} e^{-y^2/2}(2y^2 - 1) = \phi_2(y)$$

$$H_{11} = \langle u_1 | -\frac{d^2}{dy^2} + y^4 | u_1 \rangle = \frac{5}{4}$$

$$\epsilon \begin{vmatrix} C_1 \\ C_2 \end{vmatrix} = \begin{bmatrix} \frac{5}{4} & \sqrt{2} \\ \sqrt{2} & \frac{49}{4} \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$$

$$E_t \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} H_1 & H_{12} \\ H_{21} & H_{22} \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$$

$$\begin{bmatrix} H_{11} - E_t & H_{12} \\ H_{21} & E_{22} - E_t \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = 0$$

$$\det \begin{vmatrix} H_{11} - E_t & H_{12} \\ H_{21} & E_{22} - E_t \end{vmatrix} = 0$$

$$(H_{11} - E_t)(H_{22} - E_t) - H_{12}H_{21} = 0$$

Random idea:

make python implementation of mathmatica

$$E_{\pm} = \frac{27 \pm 2\sqrt{129}}{4}$$

$\psi_t = 0.99209\, u_1(y) + 0.1255 u_2(y)$

I might've implemented the wrong

3. basis states

$\psi_t = c_1\phi_0 + c_2\phi_2 + c_3\phi_4$

$$E \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 5/4 & \sqrt{2} & \sqrt{3}/2 \\ \sqrt{2} & \frac{49}{4} & 6\sqrt{2} \\ \sqrt{3}/2 & 6\sqrt{5} & \frac{141}{4} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} \qquad E = 1.07177$$

n	$E_0(n)$
1	1.25000
2	1.07109
3	1.07077
4	1.06503
:	~~1.06045~~ ~~1.06131~~ 1.06131
:	1.06045
	1.06039
	1.06037
	:

$\psi_t(y) = c_1 u_1(y) + c_2 u_2(y)$

$= c_1 \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha y^2/2} + c_2 \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/4} \frac{1}{\sqrt{2}} e^{-\alpha y^2/2} (2\alpha y^2 - 1)$

$$E_-[\alpha] = \frac{21 + 6\alpha^3 - 2\sqrt{3}\sqrt{33 + 8\alpha^3 + 2\alpha^6}}{4\alpha^2}$$

$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$

$i\hbar \frac{d}{dt}\bar{c}(t) = \bar{\bar{H}}\,\bar{c}(t)$

$\psi(x,t) = \sum_j c_j(t) u_j(x)$

2 level System

$V(x)$

$i\hbar \frac{\partial\psi}{\partial t} = \left[\frac{\hat{p}^2}{2m} + V(x) - F(t)x\right]\psi(x,t)$

$i\hbar \frac{\partial\psi}{\partial t} = \left[\frac{\hat{p}^2}{2m} + Ax^4 - F(t)x\right]\psi(x,t)$

Think about finite Gets

$\hat{H} = \hat{H}_0 + V(t)$ $\qquad i\hbar \frac{d}{dt} \bar{c}(t) = \bar{\bar{H}}(t) \bar{c}(t)$

$E_j \phi_j = \hat{H}_0 \phi_j$

$\Psi(x,t) = \sum_i c_j(t) \phi_j(x)$

development of a approximate Hamiltonian
exact $\hat{H}$, approximate $\Psi_t(x,t)$

$\Rightarrow$ New approx. $\hat{H}_{appr.}$ exact Ψ

~~Exact $\hat{H}$, approx~~ $\hat{H} = \sum_j \sum_k |\phi_j\rangle \langle \phi_j | \hat{H} | \phi_k\rangle \langle \phi_k|$

$= \left[\sum_j |\phi_j\rangle\langle\phi_j|\right] \hat{H} \left[\sum_k |\phi_j\rangle\langle\phi_k|\right]$

$\sum_j |\phi_j\rangle\langle\phi_j| = \mathbb{1}$

$\langle\phi_j|\hat{H}|\phi_j\rangle = \langle\phi_j| \left[\sum_{j'}\sum_{k'} |\phi_{j'}\rangle\langle\phi_j|\hat{H}|\phi_k\rangle\langle\phi_{k'}|\right] |\phi_k\rangle$

$= \langle\phi_j| \left[\sum_{j'} |\phi_{j'}\rangle\langle\phi_j|\hat{H}|\phi_k\rangle \langle\phi_k|\phi_k\rangle\right.$ $\qquad \langle\phi_{k'}|\phi_k\rangle = 0$; $\underset{1}{\parallel}$ $k = k'$

$= \langle\phi_j|\phi_j\rangle \langle\phi_j|\hat{H}|\phi_k\rangle$
$\underset{1}{\parallel}$ $= \langle\phi_j|\hat{H}|\phi_k\rangle$

perturbation tickles $\rightarrow$ we want to see what the tickling does

approx. $\hat{H}_{2\,level} = \sum_{j=1}^{2}\sum_{k=1}^{2} |\phi_j\rangle\langle\phi_j|\hat{H}|\phi_k\rangle\langle\phi_k|$