P4410 LECTURE 23

Approximation methods

The class of QM problems that can be solved exactly is small — and the class of problems that can be solved without a computer is even smaller — we've already done most of them! So the next few weeks will be dedicated to the following approximation techniques that will allow us to attack a more general set of problems:

1. Variational method — a way to approximate the ground state of a bound system

2. Time-independent perturbation theory — a series expansion for the eigenvalues/eigenstates of a Hamiltonian in the case where one knows the exact solution to a very similar Hamiltonian. Example: corrections to H atom spectrum

3. Time-dependent perturbation theory — addresses situations where the Hamiltonian is perturbed and causes transitions from one state to another in time. Example: stimulated emission (e.g. lasers).

Start with the least broadly applicable: variational method. Take a Hamiltonian $\hat{H}$ that has bound states. Let $|\psi_0\rangle$ be the exact ground state. The expectation value of energy for this state is the ground state energy E_0:

$$\langle \psi_0 | \hat{H} | \psi_0 \rangle = E_0 .$$

Now take some random state $|\psi\rangle$ and evaluate $\langle E\rangle$:

$$\langle\psi|\hat{H}|\psi\rangle = E \geq E_0 .$$

One way to see this is to expand $|\psi\rangle$ in the energy basis:

$$|\psi\rangle = \alpha|\psi_0\rangle + \sum_{i=1}^{\infty}\beta_i|\psi_i\rangle$$

so $\langle\psi|\hat{H}|\psi\rangle = \alpha E_0 + \sum_i \beta_i E_i$ <u>But every E_i is greater than E_0.</u>

So this expectation value is minimized when $\alpha \to 1$ and $E \to E_0$.

Another way to show it:

$$E - E_0 = \langle\psi|\hat{H}|\psi\rangle - \langle\psi_0|\hat{H}|\psi_0\rangle = \langle\psi|\hat{H} - E_0|\psi\rangle$$

$$E - E_0 = \sum_{i,j}\langle\psi|\psi_i\rangle\underbrace{\langle\psi_i|(\hat{H}-E_0)|\psi_j\rangle}_{=(E_i - E_0)\delta_{ij}}\langle\psi_j|\psi\rangle$$

$$= \sum_i (E_i - E_0)\langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle$$

$$= \sum_i (E_i - E_0)\;|\langle\psi_i|\psi\rangle|^2 \quad \geq 0$$

where equality is achieved if $|\psi\rangle = |\psi_0\rangle$.

Conclusion: if we guess the ground state, any error will only increase the energy $\Rightarrow$ if we modify our guess and it <u>lowers</u> the energy, we know we are <u>closer</u> to the ground state.

Procedure: parametrize our guess at the state.

Let unnormalized guess $\equiv |\bar{\Psi}\rangle$ (Shankar's notation).

$$\bar{E} = \frac{\langle\bar{\Psi}|\hat{H}|\bar{\Psi}\rangle}{\langle\bar{\Psi}|\bar{\Psi}\rangle}$$

Define $|\bar{\Psi}\rangle$ in terms of parameters λ_1, λ_2, etc. Often these will be expressed in position or momentum basis (if we knew the energy basis we wouldn't need to guess!): $\langle x|\bar{\Psi}\rangle = x^{\lambda_1} e^{\frac{-x^2}{2\lambda_2}}$ etc.

So $\bar{E}$ is a function of our parameters: $\bar{E}(\lambda_1, \lambda_2, \lambda_3, \ldots)$

$\bar{E}$ is minimized when $\frac{d\bar{E}}{d\lambda_i} = 0$ for all λ_i. This is an example of a variational principle. Note that if the $|\bar{\Psi}\rangle$ actually span the Hilbert space (normally they won't) then the variational principle gives the exact ground state.

The trick in solving problems is to guess wisely. Examine the Hamiltonian for symmetries and build a test function that uses the symmetries, what you know about ground states (no nodes), and try to minimize the number of parameters.

Example: 1-D box, length a: Try $\bar{\Psi}(x) = x(a-x)$ → has right symmetry, no nodes.

$$\Rightarrow \bar{\Psi}' = a - 2x, \quad \bar{\Psi}'' = -2 \Rightarrow \bar{E}\cdot\langle\bar{\Psi}|\bar{\Psi}\rangle = \langle\bar{\Psi}|\hat{T}|\bar{\Psi}\rangle = \frac{-\hbar^2}{2m}\cdot(-2)\int_0^a dx\, x(a-x)$$

$$= \frac{\hbar^2}{m}\frac{a^3}{6} \quad \text{and} \quad \langle\bar{\Psi}|\bar{\Psi}\rangle = \int_0^a dx\, x^2(a-x)^2 = \int_0^a dx\, (x^4 - 2ax^3 + a^2x^2)$$

$$= \frac{a^5}{5} - \frac{2a\cdot a^4}{4} + \frac{a^2 a^3}{3} = \frac{a^5}{30}$$

$$\Longrightarrow \bar{E} = \frac{\langle\bar\Psi|\hat T|\bar\Psi\rangle}{\langle\bar\Psi|\bar\Psi\rangle} = \frac{\hbar^2}{m}\frac{a^3}{6}\frac{30}{a^5} = \frac{10\,\hbar^2}{2mL^2}$$

Vs exact solution $\pi^2 \frac{\hbar^2}{2mL^2}$ and π^2 is very close to 10.

Harmonic oscillator: $\hat H = \frac{1}{2}m\omega^2 x^2 + \frac{1}{2m}\hat p^2$

Try Gaussian: $\bar\Psi(x) = e^{-\frac{\alpha x^2}{2}}$ where α is variational parameter.

$$\frac{d\bar\Psi}{dx} = -\alpha x e^{-\frac{\alpha x^2}{2}} \qquad \frac{d^2\bar\Psi}{dx^2} = (-\alpha + \alpha^2 x^2) e^{-\frac{\alpha x^2}{2}}$$

so $$\langle\bar\Psi|\hat H|\bar\Psi\rangle = \int_{-\infty}^{\infty} dx \left[\frac{-\hbar^2}{2m}(-\alpha + \alpha^2 x^2) + \frac{1}{2}m\omega^2 x^2\right] e^{-\alpha x^2}$$

$$= \frac{\hbar^2\alpha}{2m} I_0(\alpha) + \left(\frac{-\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 x^2\right) I_2(\alpha)$$

and $\langle\bar\Psi|\bar\Psi\rangle = I_0(\alpha)$ where $I_n(\alpha) \equiv \int dx\, e^{-\alpha x^2} x^n$

So $I_0(\alpha) = \sqrt{\frac{\pi}{\alpha}}$, $I_2(\alpha) = -\frac{d}{d\alpha} I_0(\alpha) = \frac{\sqrt\pi}{2\alpha^{3/2}}$

$$\bar E = \frac{\hbar^2\alpha}{2m} + \left(\frac{-\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2\right)\frac{1}{2\alpha} = \frac{\hbar^2\alpha}{4m} + \frac{1}{4}\frac{m\omega^2}{4}$$

$$\frac{-d\bar E}{d\alpha} = \frac{\hbar^2}{4m} - \frac{m\omega^2}{4\alpha} = 0 \text{ when } \alpha^2 = \left(\frac{m\omega}{\hbar}\right)^2$$

$\bar\Psi(x) = \exp\left(\frac{-m\omega}{2\hbar}x^2\right)$ exact solution!