Physics 342 Lecture 33

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Welcome back for another quantum lecture on approximation! If you recall, in the previous lecture, we introduced the variational method for estimation of the ground state energy. We first observed, and subsequently proved, that for a system defined by a Hamiltonian $\hat{H}$ with ground state energy E_0, the expectation value of $\hat{H}$ on <u>any</u> state $|\psi\rangle$ is bounded from below by the ground state energy:

$\langle\psi|\hat{H}|\psi\rangle \geq E_0$. With this observation, we then constructed an ansatz for the ground state wavefunction with a set of parameters $\{\alpha_i\}$:

$$\psi \equiv \psi(x;\alpha_1,\alpha_2,\ldots,\alpha_n).$$

The name of the variational method game is to calculate the expectation value of $\hat{H}$ as a function of the parameters:

$$\langle\hat{H}\rangle(\alpha_1,\alpha_2,\ldots,\alpha_n) = \int dx\, \psi(x;\alpha_1,\alpha_2\ldots,\alpha_n)^* \hat{H}\psi(x;\alpha_1,\alpha_2,\ldots,\alpha_n)$$

and then minimize it over the parameters. In practice, this typically means taking all partial derivatives and demanding they vanish:

$$\frac{\partial\langle\hat{H}\rangle}{\partial\alpha_1} = \frac{\partial\langle\hat{H}\rangle}{\partial\alpha_2} = \cdots = \frac{\partial\langle\hat{H}\rangle}{\partial\alpha_n} = 0$$

Then, at this minimum, $\langle\hat{H}\rangle$ is as small as possible given the ansatz functional form for the wavefunction.

In this lecture, we are going to introduce yet another approximation method, called the <u>power method</u>. Its efficacy relies on the following observation regarding repeated action of <u>any</u> linear operator on a vector/state. For concreteness, consider a Hermitian matrix $\mathbb{A}$, and we will call its collection of eigenvalues $\{\vec{v}_i\}_i$ such that:

$\mathbb{A}\vec{v}_i = \lambda_i \vec{v}_i$. Further, we will assume that the eigenvalues are ordered in magnitude such that

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_i| > \cdots$$

We assume for simplicity that all eigenvalues are unique, which is why we can write strict inequalities. Now, let's consider what happens when we act matrix $\mathbb{A}$ on an arbitrary vector $\vec{u}$, a number of times. Assuming that the eigenvalues of $\mathbb{A}$ are complete, then we can express $\vec{u}$ as a linear combination of $\{\vec{v}_i\}$:

$\vec{u} = \sum_{i=1} \beta_i \vec{v}_i$, for some coefficients β_i.

Now, acting $\mathbb{A}$ on $\vec{u}$ once pulls out a factor of eigenvalues for each term:

$\mathbb{A}\vec{u} = \sum_{i=1} \beta_i \lambda_i \vec{v}_i$, and acting $\mathbb{A}$ on $\vec{u}$ n times pulls out

n factors of eigenvalues: $\mathbb{A}^n \vec{u} = \sum_{i=1} \beta_i \lambda_i^n \vec{v}_i$.

Here's the trick: as we assumed an ordering to the eigenvalues, for sufficiently large n, $\mathbb{A}^n\vec{u}$ gets closer and closer to parallel (i.e., proportional to) $\vec{v}_1$, the eigenvector with largest eigenvalue. So, given any old vector $\vec{u}$, we can get a better and better approximation to the eigenvector with largest eigenvalue, $\vec{v}_1$.

Now how does this help us with quantum mechanics, diagonalizing the Hamiltonian? Again, we want to solve

$\hat{H}|\psi\rangle = E|\psi\rangle$, for eigenstate $|\psi\rangle$ and eigen energy E.

Typically, we don't want to identify the largest eigenvalue of $\hat{H}$ or its corresponding state, and in most all cases there isn't even a largest eigenvalue. As with the variational method, we want to find the ground state, which, by definition, is the state with smallest eigenvalue of $\hat{H}$. So why do I claim this power method can help us find the ground state?

Well, here's the trick. If the Hamiltonian is invertible; i.e., has no eigenvalues of 0, then $\hat{H}^{-1}$ exists. If so, then we can multiply our traditional Schrödinger equation eigenvalue problem by $\hat{H}^{-1}$ on both sides:

$$\hat{H}|\psi\rangle = E|\psi\rangle \Rightarrow \hat{H}^{-1}|\psi\rangle = \frac{1}{E}|\psi\rangle.$$

That is, eigenstates of $\hat{H}$ are also eigenstates of $\hat{H}^{-1}$, but with eigenvalue that is inverted. So, while the ground state of $\hat{H}$ is the state with smallest eigenvalue, that same state has the largest eigen value of $\hat{H}^{-1}$! So, using our earlier observation, if we take an arbitrary state on the Hilbert space $|\phi\rangle$, acting sufficiently many times on $|\phi\rangle$ with $\hat{H}^{-1}$ will produce a state that becomes closer and closer to proportional to the ground state of $\hat{H}$. That is,

$(\hat{H}^{-1})^n |\psi\rangle \underset{\sim}{\propto} |\psi_0\rangle$, the ground state of $\hat{H}$, for sufficiently

large n. Note the proportionality; not equality: every time $\hat{H}^{-1}$ acts, it pulls out factors of eigenvalues, so even if $|\psi\rangle$ is initially normalized, $(\hat{H}^{-1})^n|\psi\rangle$ is not. However, fixing normalization is pretty trivial, so that's something we can do later.

This seems pretty cool, but the biggest challenge will be inverting the Hamiltonian in the first place. As with the variational method, I think an example can demonstrate the technique. Let's just consider our familiar infinite square well, again with $a=1$ for simplicity. That is, the potential is:

$$V(x) = \begin{cases} 0, & 0<x<1 \\ \infty, & \text{else} \end{cases}$$

In the well, the Hamiltonian is of course exclusively kinetic energy:

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, \text{ in position space.}$$

To use this power method to find the ground state, we need to determine what the inverse of this Hamiltonian is; that is

$$\hat{H}^{-1} = \frac{2m}{\hat{p}^2}, \text{ or what the inverse of the momentum operator } 1/\hat{p} \text{ is! Huh?}$$

The inverse momentum operator, $\hat{p}^{-1}$ is defined to return the identity operator when acting on $\hat{p}$. That is:

$(\hat{p}^{-1})\,\hat{p} = \mathbb{1}$, obviously. Let's work in position space and we need to introduce a test function

$f(x)$ to keep us honest about linearity of these operators. In position space, of course

$\hat{p} = -i\hbar \frac{\partial}{\partial x}$, so we want to

find the $(\hat{p}^{-1})$ such that:

$$(\hat{p}^{-1})(-i\hbar)\frac{\partial}{\partial x'} f(x') = f(x).$$

Of course, the fundamental theorem of calculus tells us that the antiderivative (i.e., indefinite integral) is the inverse of the derivative. so, we can write

$$\hat{p}^{-1} = \frac{i}{\hbar}\int^{x} dx', \text{ so that}$$

$$(\hat{p}^{-1})\,\hat{p}\, f(x) = \frac{i}{\hbar}\int^{x} dx'\,(-i\hbar)\frac{\partial}{\partial x'} f(x') = f(x), \text{ as required.}$$

As $f(x)$ was an arbitrary test function, this shows that indeed $(\hat{p}^{-1})\,\hat{p} = \mathbb{1}$, as required.

Now, for the inverse of the infinite square well Hamiltonian, we need $(\hat{p}^{-1})^2$. Just like $\hat{p}^2$, we think of $(\hat{p}^{-1})^2$ as two consecutive actions of the operator $\hat{p}^{-1}$. Thus, if $\hat{p}^{-1}$ integrates once, $(\hat{p}^{-1})^2$ integrates twice, in composition. That is,

$$(\hat{p}^{-1})^2 = \left(\frac{i}{\hbar}\right)^2 \int^{x} dx' \int^{x'} dx''.$$

To verify this, let's act on a test function $f(x)$ and with $\hat{p}^2$ on the left:

$$\hat{p}^2(\hat{p}^{-1})^2 f(x) = (-i\hbar)^2\left(\frac{i}{\hbar}\right)^2 \frac{\partial^2}{\partial x^2}\int^{x} dx' \int^{x'} dx''\, f(x'')$$

$$= \frac{\partial}{\partial x} \int^{x} dx'' f(x'') = f(x),$$ through two applications

of the fundamental theorem of calculus. Then, we have shown that:

$$\hat{p}^2 (\hat{p}^{-1})^2 f(x) = f(x) = \mathbb{1} f(x),$$ and so

indeed we have correctly identified $(\hat{p}^{-1})^2$. Finally, the inverse of the Hamiltonian of the infinite square well is:

$$\hat{H}^{-1} = \frac{2m}{\hat{p}^2} = -\frac{2m}{\hbar^2} \int^{x} dx' \int^{x'} dx'',$$ in position space.

Additionally, we have to remember that all states in the Hilbert space vanish at the end points of the well, at $x=0$ and $x=1$.

We now have our inverse Hamiltonian, so let's figure out an estimate for the ground state wavefunction. Motivated by our considerations with the variational method of last lecture, let's make the ansatz that the ground state wavefunction is:

$$\psi(x) \propto x(1-x).$$

As mentioned before, this vanishes at $x=0, 1$, and is symmetric about the center of the well, $x=1/2$. We only care about proportionality here, because we can always divide out by the normalization factor, $\langle\psi|\psi\rangle$. For this wavefunction guess, our estimate of the ground state energy E_0 is:

$$E_0 \sim \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = -\frac{\hbar^2}{2m} \frac{\int_0^1 dx\, x(1-x) \frac{\partial^2}{\partial x^2} x(1-x)}{\int_0^1 dx\, x^2(1-x)^2}$$

These integrals are easy enough to evaluate. For the numerator, we find

$$\int_0^1 dx\, x(1-x)\, \frac{\partial^2}{\partial x^2} x(1-x) = -2\int_0^1 dx\, x(1-x) = -\frac{1}{3}.$$

The denominator is:

$$\int_0^1 dx\, x^2(1-x)^2 = \frac{1}{30}.$$

Thus, the estimate of the ground state energy is

$$E_0 \sim \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = 5\frac{\hbar^2}{m}.$$ Recall that the exact value is

$$E_0 = \frac{\pi^2}{2}\frac{\hbar^2}{m} \cong (4.934802\ldots)\frac{\hbar^2}{m},$$ so we're already pretty close.

However, the power method should produce a better estimate for the ground state ~~energy~~ wavefunction and hence its energy. The power method states that

$\hat{H}^{-1}|\psi\rangle$ is closer to (i.e., at smaller angle or more parallel to) the ground state wavefunction than $|\psi\rangle$ itself. Well, let's calculate it!

We identified $\psi(x) = x(1-x)$, again not worrying about normalization. Then the action of $\hat{H}^{-1}$ on this is:

$$\hat{H}^{-1}|\psi\rangle = \frac{2m}{\hat{p}^2}|\psi\rangle = -\frac{2m}{\hbar^2}\int^x dx' \int^{x'} dx''\, x''(1-x'')$$

$$= -\frac{2m}{\hbar^2}\int^x dx'\left(\frac{(x')^2}{2} - \frac{(x')^3}{3} + c_1\right)$$

$$= -\frac{2m}{\hbar^2}\left(\frac{x^3}{6} - \frac{x^4}{12} + c_1 x + c_2\right),$$ where c_1 and c_2 are integration constants.

We fix c_1 and c_2 by demanding that $\hat{H}^{-1}|\psi\rangle$ vanishes at the boundaries of the well. $x=0$ forces that $c_2=0$ and $x=1$ forces $c_1=-1/12$. Thus, we have that

$\hat{H}^{-1}|\psi\rangle = \frac{2m}{\hbar^2}\left(\frac{x}{12}-\frac{x^3}{6}+\frac{x^4}{12}\right)$, but all we care about is

proportionality, so we just have

$\hat{H}^{-1}|\psi\rangle \propto x-2x^3+x^4$. Now with this estimate for

the ground state wavefunction, let's evaluate the estimate of the ground state energy:

$$E_0 \sim \frac{\langle\psi|(\hat{H}^{-1})\hat{H}(\hat{H}^{-1})|\psi\rangle}{\langle\psi|(\hat{H}^{-1})(\hat{H}^{-1})|\psi\rangle} = -\frac{\hbar^2}{2m}\frac{\int_0^1 dx\,(x-2x^3+x^4)\frac{\partial^2}{\partial x^2}(x-2x^3+x^4)}{\int_0^1 dx\,(x-2x^3+x^4)^2}.$$

Now, we just evaluate the integrals in the numerator and denominator. For the numerator, we have

$$\int_0^1 dx\,(x-2x^3+x^4)\frac{\partial^2}{\partial x^2}(x-2x^3+x^4) = -\int_0^1 dx\,(x-2x^3+x^4)\,12x(1-x)$$

$$= -\frac{17}{35}.$$

The integral in the denominator is

$$\int_0^1 dx\,(x-2x^3+x^4)^2 = \frac{31}{630},$$ and so our estimate for the ground state energy is:

$$E_0 \sim \left(-\frac{\hbar^2}{2m}\right)\left(-\frac{17}{35}\right)\left(\frac{630}{31}\right) = \frac{153}{31}\frac{\hbar^2}{m} \cong (4.93548\ldots)\frac{\hbar^2}{m}.$$

This differs from the exact result by about one part in

10000, which is an order of magnitude more accurate than what we predicted from the variational method!

I hope this very brief introduction into approximation methods has been fun and interesting. This is the last material that you will have regular homework on. For the last two weeks of class, we'll just have fun. :)