Physics 750: Lecture 15

Thursday, November 2, 2017

So far, our discussion of quantum mechanics has focussed on solving the Schrödinger equation for a single particle in one spatial dimension (1D). How do we adapt our numerical methods to handle the more general *many-body problem* in *higher dimensions*?

Dimensionality

1D is special because the boundary—marked, e.g., by the edges of an impenetrable potential well—consists of just two points. In 2D, the boundary is a line; in 3D a surface, etc. Hence, the shooting and matching methods are no longer very useful. Remember that if we have a quantum particle confined to the line segment $[0, L]$, then we can assume $\psi(0) = 0$ and $\psi'(x) = \epsilon$. The value of ϵ is fixed after the fact by imposing the normalization condition $\int dx\, |\psi(x)|^2 = 1$. Given a guess value for the energy E, we can integrate to the right edge of the well and use the roots of $g(E) = \psi(L)$ to determine the eigenenergies.

In 2D, we can chose an arbitrary point on the boundary with $\psi(x_0, y_0) = 0$, but the initial values of the spatial derivatives in *two* orthogonal directions, $\psi_x(x_0, y_0) = \epsilon_x$ and $\psi_y(x_0, y_0) = \epsilon_y$, have to be specified. The eigenstates now correspond to the roots of

$$g(E, \epsilon_x, \epsilon_y) = \int_{\text{boundary}} d^2r |\psi(x, y)|^2.$$

One free parameter is removed by fixing the normalization, but this is still a root-finding problem in a two-dimensional space. (Quite tricky, because we no longer have an intermediate value theorem to bracket the roots!) There's also the difficulty that the points in a simple, orthogonal spatial grid may not align with the boundary; on the other hand, a grid adapted to the boundaries will required a more careful treatment of the finite differences.

Multiple particles

In the case of N particles living in a D-dimensional space, the wavefunction of the system

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$$

is a function of $N\,D$ real variables. The Hamiltonian can now have many-body interaction terms:

$$\hat{H} = \sum_i \left(-\frac{\nabla^2}{2m_i} + V(\boldsymbol{r}_i) \right) + \sum_{i<j} U(\boldsymbol{r}_i - \boldsymbol{r}_j).$$

Another complication is that the particles will have either fermionic or bosonic "statistics," meaning that they may or may not experience a π phase shift when two particles are exchanged. That is to say,

$$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_i, \ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_N) = \mp \Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_i, \ldots, \boldsymbol{r}_N).$$

Any solution you generate must be properly (anti)symmetrized.

Matrix mechanics

In most cases, and especially when there are strong interactions between particles, it is not simple to solve the Schrödinger equation. So far, our strategy has been to solve for the energy eigenstates, expand the $t = 0$ snapshot $\psi(x, 0)$ in that basis, and compute $\psi(x, t)$ based on the $e^{-iE_n t/\hbar}$ phase evolution in each mode. In general, though, finding the eigenstates is nontrivial.

Even if we don't have access to the eigenstates, we can always concoct a complete set of wavefunctions to serve as a basis. Now suppose we have a complete set $\{\phi_n\}$ that is finite, or at the very least *countably* infinite. Then we define a matrix $H_{n,m}$ and a vector ψ_n according to

$$H_{n,m} = \langle n|\hat{H}|m\rangle = \int d^3r\, \phi_n(\boldsymbol{r})^* \hat{H} \phi_m(\boldsymbol{r})$$
$$\psi_n = \langle n|\psi\rangle = \int d^3r\, \phi_n(\boldsymbol{r})^* \psi(\boldsymbol{r})$$

Inserting the completeness relation $\sum_n |n\rangle\langle n| = 1$ into $\hat{H}|\psi\rangle = E|\psi\rangle$ gives

$$\begin{aligned} E\psi_n = E\langle n|\psi\rangle &= \langle n|\hat{H}\left(\sum_m |m\rangle\langle m|\right)|\psi\rangle \\ &= \sum_m \langle n|\hat{H}|m\rangle\langle m|\psi\rangle = \sum_m H_{n,m}\psi_n. \end{aligned} \tag{1}$$

This is just the matrix eigenvalue problem

$$\begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & \ddots & \\ \vdots & & \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$$

This system of equations has solutions whenever the characteristic polynomial $\lambda(E) = \det(H - E)$ vanishes. For each root $E^{(\alpha)}$, there is a corresponding eigenvector $\psi_n^{(\alpha)}$. If the size of the matrix is not too unmanageable, then the eigenvalue problem can be solved numerically using, e.g., LAPACK routines. This is called *exact diagonalization*. Under the appropriate unitary transformation,

$$U^\dagger H U = \begin{pmatrix} E_0 & & \\ & E_1 & \\ & & \ddots \end{pmatrix}$$

But for many-body problems, the size of the Hilbert space usually grows exponentially in the number of particles, so a direct solution is not always practical. Nonetheless, it may be that you don't need to know all the eigenstates. For example physical properties at low temperatures ($T \ll E_1 - E_0$) are dominated by the ground state (the eigenstate of lowest energy).

Here we outline the *power method* for finding the ground state. Choose a constant C large enough so that all the diagonal terms $\tilde{E}_n = E_n - C$ in the matrix $U^\dagger H U - CI$ are strictly negative. Pick a trial state $\psi^{(0)} = \sum_n c_n^{(0)}\phi_n$ expressed as an expansion in the (as yet unknown) energy eigenstates. An improved estimate is given by

$$\psi^{(1)} = (C - U^\dagger H U)\psi^{(0)} = \sum_n c_n^{(0)}(C - E_n)\phi_n.$$

This can be done iteratively:

$$\begin{aligned} \psi^{(k)} &= \sum_n c_n^{(0)}(C - E_n)^k \phi_n \\ &= (C - E_0)^k \left[c_0^{(0)}\psi_0 + c_1^{(0)}\left(\frac{C - E_1}{C - E_0}\right)^k \phi_1 + c_2^{(0)}\left(\frac{C - E_2}{C - E_0}\right)^k \phi_2 + \cdots\right] \end{aligned}$$

Note that all but the first term vanish in the large k limit:

$$\lim_{k\to\infty}(C - U^\dagger H U)^k \psi^{(0)} = \phi_0.$$

But is this useful? We don't know the transformation U. It turns out, that doesn't matter. Since $C - U^\dagger H U = U^\dagger (C - H) U$, we can invert the transformation and show that the power method yields the ground state in whatever basis we work in:

$$\lim_{k\to\infty} (C - H)^k (U\psi^{(0)}) = U\phi_0.$$

A related but slightly different set of algorithms goes under the name *Lanczos methods*.

Variational principle

The ground state $|\psi_0\rangle$ satisfies $\hat{H}|\psi_0\rangle = E|\psi_0\rangle$. Hence, the exact equality

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

holds. It is also true that for any arbitrary wavefunction obeys the inequality

$$E_0 \leq \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}.$$

In other words, the true ground state energy E_0 forms an absolute lower bound on the energy expectation value of any state. We can show this as follows. Express $\psi = \sum_n c_n \phi_n$ in the basis of energy eigenstates. Then

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \sum_{n,m} c_n^* c_m \langle\phi_n|\hat{H}|\phi_m\rangle \\
&= \sum_{n,m} c_n^* c_m E_n \delta_{n,m} \\
&= \sum_n E_n |c_n|^2 \\
&\geq E_0 \sum_n |c_n|^2 = E_0 \langle\psi|\psi\rangle.
\end{aligned}$$

This means that $E[\{c_n\}]$ defines a complicated energy landscape (with dimension equal to the rank of the Hamiltonian matrix), whose global minimum corresponds to the ground state.

In situations where the Hilbert space is too large, the optimization problem becomes intractable. In that case it may be better to work with a smaller set of physically-motivated states $\{\chi_1, \ldots, \chi_M\}$ with $M \ll \dim(H)$. The trial wavefunction $\psi = \sum_{m=1}^{M} \alpha_m \chi_m$ can be optimized by finding the global minimum in the more manageable $E[\{\alpha_m\}]$ landscape. The extremal state is no longer guaranteed to be the true ground state, but so long as the $\{\chi_m\}$ are well chosen, it may be a very good approximation to the ground state.