XI. RAYLEIGH-RITZ VARIATIONAL METHOD

Let's take a detour before approaching the two delta's problem. This detour brings us to chapter 7 of Griffiths. As it turns out, there is a simple way of obtaining pretty good estimates for the ground state of the SE without much effort. The idea is simple: make a guess as to what the solution looks like, and allow it some freedom. Calculate the expectation value of the energy under your assumption, and minimize it under the possible parameters.

Let's see why this works. The hamiltonian is a hermitian operator, and it is bounded from below. Therefore there always exists a ground state energy E_G such that:

$$\hat{\mathcal{H}} = \sum_n E_n \left|n\right\rangle \left\langle n\right| \tag{271}$$

with E_n increasing with n, and $E_n \geq E_0 = E_G$. Could you think of any vector in the Hilbert space which will give an expectation value for the energy which is less then E_G? That's clearly impossible. Let's quickly prove it. Assume a normalized vector $\left|v\right\rangle$ is your candidate. By the fact that the eigenstates of $\hat{\mathcal{H}}$ are a spanning basis, we know we can break $\left|v\right\rangle$ into a sum in terms of $\left|n\right\rangle$. Then:

$$\left|v\right\rangle = \sum_{n=0}^{\infty} c_n \left|n\right\rangle \tag{272}$$

with $\sum\limits_n |c_n|^2 = 1$. Now it becomes easy to calculate the expectation value of the energy:

$$\left\langle v\right| \hat{\mathcal{H}} \left|v\right\rangle = \sum_{n=0}^{\infty} E_n |c_n|^2 \tag{273}$$

This is an average of the energy eigenvalues with relative probability $|c_n|^2$. It can not be smaller than the smallest element - E_0!

This is an honest to God theorem. This theorem suggests a way for constructing solutions for the SE. We can make an educated guess for $\left|v\right\rangle$ which will depend on various parameters. The more parameters you have, the more you can minimize, and the closer you get to the ground state energy. The only problem is that you never know how close you really are.

A quick example: Consider the hamiltonian for a harmonic oscillator:

$$\hat{\mathcal{H}} = -\frac{1}{2}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2. \tag{274}$$

Let's find its ground state variationally. Now, this is not so fair since we already know what the ground state looks like: A Gaussian. But even if we hadn't known that, we would probably still guess the same thing. So given the benefit of the doubt, and my advanced age and declining computational skills, let's work out this example choosing a Gaussian as our variational ansatz:

$$\left|\psi_b\right\rangle = N e^{-\frac{bx^2}{2}} \tag{275}$$

We must have the Gaussian normalized:

$$\int dxpsi^2 = \int dx N^2 e^{-bx^2} = N^2\sqrt{\pi/b} = 1 \tag{276}$$

Having this to define our N, the next step is to calculate the expectation value of the Hamiltonian with this wave function:

$$E(b) = \left\langle \psi_b\right| \hat{\mathcal{H}} \left|\psi_b\right\rangle \tag{277}$$

This integral has two pieces. The spring constant piece:

$$\int dx N^2 e^{-bx^2}\frac{1}{2}kx^2 = \frac{N^2}{2}k \cdot \frac{1}{b^{3/2}}\int dy y^2 e^{-y^2} \tag{278}$$

where we introduced the rescaled variable $y = \sqrt{b}x$. The second term is:

$$-\frac{\hbar^2}{2m}\int dx N^2 e^{-bx^2/2}\frac{\partial^2}{\partial x^2}e^{-bx^2/2} \tag{279}$$

Notice how this operates on just one of the wave functions. We can correct that in favor of a more egalitarian distribution of the operators using - you got it, integration by part!

$$= \frac{\hbar^2}{2m}N^2 \int dx \frac{\partial e^{-bx^2/2}}{\partial x}\frac{\partial e^{-bx^2/2}}{\partial x} = \frac{\hbar^2}{2m}N^2 \int dx e^{-bx^2} b^2 x^2 \tag{280}$$

and again using the rescaling trick we have:

$$= \frac{\hbar^2}{2m}N^2 \sqrt{b} \int dy e^{-y^2} y^2 \tag{281}$$

And we get the following expression for the total energy:

$$E(b) = \int dy e^{-y^2} y^2 \frac{1}{\sqrt{\pi}} \left(\frac{\hbar^2}{2m} b + \frac{k}{2}\frac{1}{b} \right) \tag{282}$$

This clearly has a minimum with respect to b:

$$0 = \frac{\partial E(b)}{\partial b} = C \left(\frac{\hbar^2}{2m} - \frac{k}{2}\frac{1}{b^2} \right) \tag{283}$$

and we lumped all the integrals and constants in front into the super constant C. The answer is staggeringly simple:

$$b = \frac{\sqrt{km}}{\hbar} \tag{284}$$

Please check to see whether this fits the ground state.

Now, if you want the value of the ground state energy, we just substitute the answer for b (and do the integral...) and we get:

$$E(b_{min}) = \frac{1}{2}\hbar\sqrt{\frac{k}{m}}. \tag{285}$$

We didn't need to solve a single differntial equation... Of course, we had some prior knowledge! We restricted ourselves to functions that looked reasonable, and we got a good answer. It turns out that it is easy to get a good answer to the energy even when the wave function is not so great.

A. The variational method for a subspace of the Hilbert space

Let's think of the variational method using the bra-ket formalism and a linear algebra notation. Suppose that instead of putting parameters deep in the definining properties of some functions, we decide to consider a possible superposition of some known and liked kets:

$$\{|\phi_n\rangle\}_{n=1}^{N} \tag{286}$$

This is a finite set of some vectors we really like. Now, we would like to write up the best ground state we can get in this set for an Hamiltonian $\hat{\mathcal{H}}$.

What do we need to do? First, let's write down the most general wave function in this space:

$$|psi\rangle = \sum_n c_n |\phi_n\rangle \tag{287}$$

What's next? We need to calculate the expectation value of the energy, and minimize it:

$$E_c = \frac{\langle\psi| \hat{\mathcal{H}} |\psi\rangle}{\langle\psi|\,\psi\rangle} \tag{288}$$

We must not forget the normalization - it is really crucial here. This is written then as:

$$E_c = \frac{\sum\limits_{n,m=1}^{N} c_n^* c_m \langle\phi_n| \hat{\mathcal{H}} |\phi_m\rangle}{\sum\limits_{n=1}^{N} c_n^* c_n} \tag{289}$$

To minimize this energy, we need to minimize with respect to all variables. In this case, this entails differentiating with respect to all c's. Acatually, we can also just differentiate with respect to all c^*'s - It'll give a nicer final result. Let's see:

$$\frac{\partial E_c}{\partial c_n^*} = \frac{\sum_{n1}^{N} \langle \phi_n | \hat{\mathcal{H}} | \phi_m \rangle c_m}{\sum_{n=1}^{N} c_n^* c_n} - \frac{\langle \psi | \hat{\mathcal{H}} | psi \rangle}{\langle \psi | \psi \rangle} \frac{c_n}{\langle \psi | \psi} = 0 \tag{290}$$

This looks like a mess at first site, but really what we have after canceling the $\langle \psi | \psi \rangle$ is:

$$\sum_{m=1}^{N} \hat{\mathcal{H}}_{nm} c_m = E_c c_n \tag{291}$$

Looks familiar? How can we solve this? We need to find the set of numbers $\{c_m\}$ which is an eigenstate of the *restricted hamiltonian* $\hat{\mathcal{H}}_{nm} = \langle \phi_n | \hat{\mathcal{H}} | \phi_n \rangle$. The energy would be E_c, the ground state. Needless to say, there might be many answers - in fact, N of them (as many as the parameters we have). The lowest one will be the ground state. But it'll come to you at no surprise, that the other solutions will be an approximation for the excited states.