

Advanced Quantum Mechanics with Applications
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Lecture – 24

Variational method, Variation of constants, Upper bound on ground state energy

So, now we shall discuss another approximate methods in context of the ongoing discussion which is called as a Variational method.

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Variational Method

$H = H_0 + H'$ ← we don't know how to do this split.
 H is known but not its decomposition into H_0 & H' .
 The solution of H is not known.

$H|\phi_n\rangle = E_n|\phi_n\rangle \quad |\psi\rangle = \sum_n a_n|\phi_n\rangle$

$\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$

The choice of $|\psi\rangle$ should be such that
 $\langle H \rangle \geq E_0$ E_0 : actual ground state energy.
 smallest e -value of H .

And this method has found its use in a variety of situation including a number of research problems such as the quantum hall effect or even the BCS theory which is known to be a theory of superconductivity which is due to burdening cooper and schrieffer and the first microscopic theory on superconductivity is actually a variational theory. And as I said that it has been really helpful in a variety of situations particularly when you do not know how to distinguish a Hamiltonian in terms of its unperturbed and it is perturbed or perturbation components. So, we do not know how to do this which means that.

So, we know the Hamiltonian H is known, but not its decomposition or decoupling rather whatever you want to call them is decomposition into H_0 and H' . So, as a result the solution of H is not known. So, just recognize that this is a different class of problems as compared to the perturbation theory that we had seen where there was a clear

demarcation of what is the perturbation Hamiltonian because a number of the corrections were computed in terms of the H' the matrix elements of H' .

So, a knowledge of H' exact knowledge of H' how it looks like what are the dependencies on various parameters relevant to the problem that was a crucial input in that case while that input may not be available. You simply know that there is a Hamiltonian which need to be solved and there is no exact solution that is possible of course, because had there been an exact solution, then none of the approximate methods would have been required. So, we are in a situation in which we have H the solution of H is not known and needs to be ascertained and neither H can be split into H_0 and an H' .

Formally of course, one can always write down the H of you know say ψ_n its equal to $E_n \psi_n$. Because whatever the solutions are where ψ is the solution which is equal to say $\sum_n a_n \psi_n$. This is a very important postulate in quantum mechanics that is the total wave function is written in terms of the basis states and I just to tell you that what basis states are. If I simply write down matrix without specifying what the matrix of the x and the y columns they stand for, the matrix should not have any meaning to you.

So, I will have to say that this corresponds to the registration number that is the in the x direction the registration number of candidates and in the y direction we have noted down the numbers you have gotten for this particular case and in which case now you know that we are or rather a number of courses that you have taken particularly this semester.

So, in a particular case one student has got one number and then, you know that this table or the matrix which has been supplied to you makes sense. This knowledge of what is plotted versus what or what are the registration number of the role number of candidates and the basically all these courses or the you know the classification of various courses that you are doing is the basis for this problem.

So, in the same way we need a basis just to get you back to this problem of spin half, then we had a basis of up and down or 1 and 0 where the base seen in the context of quantum computation in principle that basis could be infinite as we have seen. However, for use I mean particular applications, you could have a basis of different sizes. If this

you have an infinite basis for a given problem then that vector space or the set of all the basis functions is called as a Hilbert space and. So, this n actually goes from some 0 to infinity or 1 to infinity and this ϕ_n s are the basis functions.

If you need to have in a given case if you need to have a time evolution of a system that time evolution is passed on to these coefficients. These coefficients as you know are in general complex, but the basis functions are left alone and they are not taken to be a time dependent that is the easiest approach.

Now, suppose we do not know ψ , but still formally we can write down the expectation value of H can be written as $\langle \psi | H | \psi \rangle$ divided by $\langle \psi | \psi \rangle$ maybe we were not writing it this ψ overlap or the inner product of ψ in most of the situations earlier. Because the understanding is that the ψ that we work with is normalized and if it is normalized, then the inner product of ψ is equal to 1 with itself. And if it is equal to one then you do not need to write it, but here we need to write it because we do not know what is the actual wave function.

So, the choice of ψ should be such that the expectation value of H is forms the upper bound of the actual ground state energy. So, the actual ground state energy the expectation value of the Hamiltonian obtained from these ψ which will just elaborate what this size are we are calling we will call this as trial states and so, on. So, the expectation value within the trial states can never give values which are more than or rather which are lower than the actual ground state.

So, they will always give values which are greater than this actual ground state whereas, So, basically that is the ground state energy means smallest eigenvalue of H . Let us prove this inequality.

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lets prove the inequality,

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle$$

$$\langle \psi | \psi \rangle = \sum_{nm} a_n a_m \underbrace{\langle \phi_n | \phi_m \rangle}_{\delta_{nm}} = \sum_n |a_n|^2$$

$$\langle \psi | H | \psi \rangle = \underbrace{\sum_n |a_n|^2 E_n}_{|a_0|^2 E_0 + |a_1|^2 E_1 + \dots} \geq E_0 \sum_n |a_n|^2$$

For this inequality to become equality, all a_n 's need to be zero, except for C_0 .

$|\psi\rangle$ is an eigenvector of H with eigenvalue E_0 .

Let ψ be that is your ψ that is the answers that you have made. ψ is equal to sum over n $a_n |\phi_n\rangle$ which is equal to sum over n $|a_n|^2$ because of the reason that these form a complete set of states which tells you that these are orthonormal to each other and that is why this will be a Kronecker delta. If the so, there is a δ_{nm} will be simply sum over n $|a_n|^2$. So, $\langle \psi | H | \psi \rangle$ which is equal to a summation over n $|a_n|^2 E_n$ has to be always greater than $E_0 \sum_n |a_n|^2$. Because this is like a $0^2 E_0 + 1^2 E_1 + \dots$ on.

So, if you take only the E_0 , this sum has to be certainly greater than E_0 . And for this inequality to become equality, we would have the all the other all a_n 's need to be 0 except for C_0 . So, ψ is an eigenvector in which case ψ will be an eigenvector of H with eigenvalue E_0 . Of course, that you have to be enormously lucky in order to get exactly the ground state energy starting from a trial function. Let us see what we mean by a trial function.

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Formulation of the variational problem.

Choose a family of states $|\psi(\alpha)\rangle$ for several choices of α .

Calculate $\langle H(\alpha)\rangle = \langle \psi(\alpha) | H | \psi(\alpha)\rangle = E_n(\alpha)$

Now minimize $\frac{dE_n(\alpha)}{d\alpha}$ and put equal to zero.

$\frac{dE_n(\alpha)}{d\alpha} = 0 \Rightarrow$ will yield a choice of α for which we obtain an upper bound on the energy.

Variational method in general can be generalized to evaluate the upper bound on energy of any excited state.

Suppose we know:

$ \psi_0\rangle$	\rightarrow	E_0	} upper bounds.
$ \psi_1\rangle$	\rightarrow	E_1	
$ \psi_2\rangle$	\rightarrow	E_2	

Formulation of the variational problem; so, let us consider choose a family of states given as $\psi(\alpha)$, so, basically for several choices of α . So, for each choice of α , we choose a ψ of α and the important thing is that α is a constant. But will still vary that constant vary means we will change that constant and calculate $H(\alpha)$; α is called as a variational parameter. So, calculate H of α by which is equal to ψ of α $H \psi$ of α which of course, gives us E of α .

So, this is if you are talking about so, this E_n of α . Now minimize $dE_n/d\alpha$ and put equal to 0. So, $dE_n/d\alpha = 0$ will give value will yield a choice of α for which the or rather for which we obtain an upper bound upper bound on the energy.

In principle we most of the time we look for the ground state energy, but it may not be the ground state we could actually get the excited state energies as well. So, a variational method to evaluate the upper bound on energy of any of the excited states. So, suppose we know ψ_0 or say ψ_0 which is the ground state which corresponds to E_0 . If we know ψ_1 , we can get an upper bound on E_1 also and ψ_2 that is the second excited state, we can get an upper bound on E_2 and so, on.

So, just to reiterate and summarize that you take a family of functions which are trial functions for you which has one variational parameter or maybe more than one variational parameter. Try to understand that the number of variational parameters being

minimum is what is desirable because ultimately you have to extremize that function or rather minimize that function put that equal to 0.

Now, finding an a minimum of a function which has two variational parameter or three variational parameters etcetera are doable. But they come with a baggage of difficulties such as you know it has to be self consistently computed that you should not get a minimum for in one corresponding to one variational parameter and come out of the minimum of the other variational parameter and so, on. So, in our discussion mostly, we are going to talk about one variational parameter. Though BCS theory by itself was originally formulated as a as a consisting of two variational parameter; however, there was a relationship between the two which yielded a single parameter variational theory.

So, in principle it can also be applied to the excited states and we will again give the upper bounds to the all the excited state energies. Most of the time we are only in search of the ground state wave function and things like that. So, let us write down.

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let us construct a set of known functions
 $|\psi_n\rangle = a_n |\phi_n\rangle$ $\{\phi_n\}$ form a complete set.
 let us trial wavefunction, $|\psi_T\rangle$ denote the ones which
 have been left out of the actual wavefunction $|\psi\rangle$
 $|\psi_T\rangle = |\psi\rangle - \sum_n a_n |\phi_n\rangle$
 $a_n = \langle \psi | \phi_n \rangle$
 $|\psi_T\rangle = |\psi\rangle - \sum_n \langle \phi_n | \psi \rangle |\phi_n\rangle$
 All the known eigenstates are orthogonal to $|\psi_T\rangle$.

Let us construct a set of functions known functions ψ_n which is equal to an ϕ_n these ϕ_n form a complete set which means they are orthonormal.

Let the trial wave function ψ_T denote the ones which have been left out left out of the actual wave functions ψ . So, that we can write down ψ_T is equal to ψ minus an ϕ_n . So, that is so, the coefficients a_n can be written as $\langle \psi | \phi_n \rangle$. So, that the ψ_T can

be written as a psi minus sum over n a phi n psi and a phi n here.. So, we can check that all the known Eigen states are orthogonal to this trial wave function all right.

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$$\begin{aligned}
 \langle \psi_T | H | \psi_T \rangle &= \langle \left(\psi - \sum_{j=0}^{\infty} a_j |\phi_j\rangle \right) | H | \left(\psi - \sum_{k=0}^{\infty} a_k |\phi_k\rangle \right) \rangle \\
 &= \langle \left(\sum_{j=n+1}^{\infty} a_j |\phi_j\rangle \right) | H | \left(\sum_{k=n+1}^{\infty} a_k |\phi_k\rangle \right) \rangle \\
 &= \sum_{j,k} a_j^* a_k E_k \underbrace{\langle \phi_j | \phi_k \rangle}_{\delta_{jk}} \\
 &= \sum_{j=n+1}^{\infty} |a_j|^2 E_j \\
 &\geq E_{n+1} \sum_{j=n+1}^{\infty} |a_j|^2 \\
 &\geq E_{n+1} \langle \psi_T | \psi_T \rangle \\
 E_{n+1} &\leq \frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}
 \end{aligned}$$

So, then of course, we can calculate psi T, there is a trial function and H and the psi T which is equal to a psi minus j equal to 0 to n where. In fact so, this is this is important here. So, so this is sorry psi minus not here. So, this is psi minus a aj phi j aj phi j. So, this is this is there and then there is a H and then there is another psi minus j equal to 0 to n and or maybe just use an another. So, this is K and a k phi K and so on.

So, this is nothing, but equal to. So, because we are taking that difference that is what is left out is j equal to n plus 1 to infinity a j phi j that is what by definition and H and similarly k equal to n plus 1 to infinity and a K phi K and like this. So, this is nothing, but j and a K a j star a K E K and there is a phi j phi K which is nothing, but a chronicle delta because of the definition we have already said that they form a complete set of states.

So, this is equal to j equal to n plus one to infinity a j mod square E j and which is nothing, but of course, greater than E n plus one j equal to n plus 1 to infinity and a phi j square. And this is of course, E n 1 and psi T psi T which is of course, equal to so, E n 1 E n plus 1 is less than equal to a psi t H psi T and psi T psi T.

So, that is the proof that any of the excited states also be computed or it is this maximum value is obtained from a variational theory. Let us see a few demonstrative examples.

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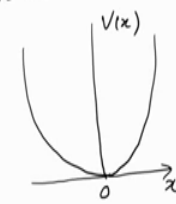
Example $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$ $K = m\omega^2$

Known results: $E_n = (n + \frac{1}{2}) \hbar \omega$
 $\psi_n = A_n H_n(\alpha x) e^{-\alpha x^2}$

$|\psi(\alpha)\rangle = e^{-\alpha x^2} \quad \alpha > 0.$

$\langle \psi(\alpha) | \psi(\alpha) \rangle = \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx$

$\langle H(\alpha) \rangle = \frac{\langle \psi(\alpha) | H | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle}$



So, let us take a one dimensional harmonic oscillator given by this. So, that is the one dimensional harmonic oscillator and suppose we do not know how to solve it. Of course, now we know how to solve it. There are complicated differential equations which people have solved in order to obtain the solution of this which we know that the let me just the known results which you should know is that the energy spectrum is given by n plus half \hbar cross ω and the wave functions are given by. So, this is some normalization constant and this is a polynomial α is some constant in terms of the m ω and k of the problem where m and K ω you are seeing. So, this is m ω square. So, K equal to m ω square.

So, basically that and then there is a Gaussian ok. So, α is in terms of m and ω and things like that. So, these are sort of solutions of this and just two. So, this is the potential. So, this is x and this is V of x . Now you see that this potential is perfectly symmetric about x equal to 0. Suppose the origin or the minimum of that potential is at x equal to 0, it is perfectly symmetric the Hamiltonians having similar symmetries are safe to have or rather these are called the parity symmetries or parity is conserved and in which case the Hilbert space or the vector space of this particular problem splits into even functions and odd functions. And these H_n these H_n αx , these are

polynomials. These polynomials are called as Hermite polynomials. These hermite polynomials have the property that when n is even it is even when n is odd it is odd.

And the other feature of this harmonic oscillator is that in usually in other cases you have seen such as hydrogen atom or particle in the box n starts from 1 to 3. Here n can assume a value 0 which is a very well a valid solution. So, H_0 here or a 0 here is a valid solution. So, the lowest energy is equal to E_0 which is half \hbar cross omega and then the energy levels are equally spaced which are we have seen in while we before we have actually started talking about the coherent states. And the squeezed states we have looked at the properties of the harmonic oscillator and they are equal equally spaced and because of this equal spacing. One could actually talk about this creation and annihilation operator and can formulate the entire problem of harmonic oscillator quantum harmonic oscillator in terms of those.

So, that part is of course, known. Suppose we do not know how to solve this the Hamiltonian and let us take an uncharged that psi alpha is simply a Gaussian for alpha to be positive. So, what is psi alpha psi alpha? That is the normalization. This is equal to exponential minus 2 alpha x square from minus infinity to plus infinity. Here make sure that we are in the regime of minus infinity to plus infinity and dx and so, your $H\psi_\alpha$ equal to psi alpha H psi alpha divided by psi alpha psi alpha and so on.

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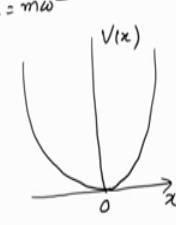
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So, the numerator can be evaluated. So, the numerator is equal to $\psi^\dagger H \psi$. So, this is equal to $\int_{-\infty}^{\infty} \psi^\dagger H \psi dx$. So, this is equal to $\int_{-\infty}^{\infty} \psi^\dagger \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi dx$. And if you calculate it becomes equal to $\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^\dagger \frac{d^2 \psi}{dx^2} dx + \frac{1}{2} m \omega^2 \int_{-\infty}^{\infty} \psi^\dagger x^2 \psi dx$. And so on. This is nothing, but $\psi^\dagger H \psi$. So, basically if this is nothing, but the denominator. So, H is equal to H which will cancel of course, with the denominator and we will have $m \omega^2$ by 8α . If you take $\frac{d}{dx} \psi = 0$, you would get α equal to $\frac{m \omega}{2 \hbar}$.

So, if you use this value of α now $2 \hbar$. So, put α back. So, put this α back into this equation and one would get H equal to $\frac{1}{2} \hbar \omega$ which in this case is exactly same as the ground state energy as we just saw here n equal to 0 is $\frac{1}{2} \hbar \omega$. And the reason that one has been able to hit the bulls eye that is get the exact ground state energy is because one has taken the exact wave function as well without the of course, the normalization the normalization has anyway being taken care of by the denominator. And because of this we can get this exactly the same this thing.

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1st excited state $|\psi\rangle = x e^{-\alpha x^2}$
 $\langle H \rangle = \frac{3}{2} \hbar \omega. \Rightarrow$ Again we have exact energy.
 Check $|\psi\rangle = \alpha x$
 $= x(\alpha^2 - x^2)$
 Calculate $\langle H \rangle.$

In fact, you can also try that because the first excited state can be also taken. We now you know for the first excited state it is actually odd.

So, we can take it as an odd function because when it change x exchanges sign this changes sign is well. If you do that then of course, you get H which is again follow the same procedure you would get H to be equal to $3 \text{ half } h \text{ cross } \omega$ which is again the exact energy.

So, just to make sure that we understand what we are talking about these ψ is the wave functions as a function of if their functions of the variational parameter. But they have to obey certain boundary conditions or certain conditions which are really the defining conditions for that problem like in the harmonic oscillator, we have taken it as a this Gaussian which is exponential minus αx^2 that turned out to be the exact one and that is why we got the exact ground state energy.

Similarly, we have applied the condition that the first excited state should be an odd function and we have made this as an odd function. You can simply use $x \psi$ equal to αx with α is the variational parameter and can check that what would be the ground state energy. So, I will write here check ψ to be equal to x or αx and equal to you know things such as x , then you have $\alpha^2 - x^2$ something like that anything that has a variational parameter and also changes sign as exchanges sign. And then calculate H and see that where you land up with.