Physics 8.321, Fall 2021
Homework #5

Due **Friday, November 5** by 8:00 PM.

1. Define the *coherent state* $|\phi\rangle = e^{\phi a^\dagger}|0\rangle$, where ϕ is a complex number, $a^\dagger$ is the creation operator for a harmonic oscillator, and $|0\rangle$ is the oscillator ground state. Show that $|\phi\rangle$ has the following properties:

(a) $|\phi\rangle = \sum \frac{\phi^n}{\sqrt{n!}}|n\rangle$

(b) $a|\phi\rangle = \phi|\phi\rangle$

(c) $\langle\phi|\phi'\rangle = e^{\phi^*\phi'}$

(d) $\langle\phi| : A(a^\dagger, a) : |\phi'\rangle = e^{\phi^*\phi'}A(\phi^*, \phi')$,
where $: A(a^\dagger, a) :$ is "normal ordered" so that all creation operators $a^\dagger$ are to the left of all annihilation operators a. You may assume that the function $A(x, y)$ can be expressed as a power series in the arguments x, y (don't worry about convergence)

(e) $\int \frac{d\phi^* d\phi}{2\pi i} e^{-\phi^*\phi}|\phi\rangle\langle\phi| = \mathbb{1}$. (completeness for coherent states)

Answer:

(a)

$$\begin{aligned}|\phi\rangle &= e^{\phi a^\dagger}|0\rangle \\ &= \sum_n \frac{(\phi a^\dagger)^n}{n!} \\ &= \sum_n \frac{\phi^n}{\sqrt{n!}}\left(\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle\right) \\ &= \sum_n \frac{\phi^n}{\sqrt{n!}}|n\rangle\end{aligned}$$

(b)

$$a|\phi\rangle = \sum_n \frac{\phi^n}{n!}a|n\rangle = \sum_n \frac{\phi^n}{n!}\sqrt{n}|n-1\rangle = \phi|\phi\rangle$$

Alternatively, you can compute $[a, e^{\phi a^\dagger}] = \phi e^{\phi a^\dagger}$. Then $a|\phi\rangle = ae^{\phi a^\dagger}|0\rangle = (e^{\phi a^\dagger}a + \phi e^{\phi a^\dagger})|0\rangle = \phi|\phi\rangle$.

(c)

$$\begin{aligned}\langle\phi|\phi'\rangle &= \langle\phi|\sum_n \frac{\phi'^n(a^\dagger)^n}{n!}|0\rangle \\ &= \langle\phi|\sum_n \frac{\phi'^n(\phi^*)^n}{n!}|0\rangle \quad \text{use conjugate of (b)} \\ &= e^{\phi^*\phi'}\langle\phi|0\rangle \\ &= e^{\phi^*\phi'}\end{aligned}$$

(d) A general term $(a^\dagger)^n a^m$

$$\underbrace{\langle\phi|(a^\dagger)^n}\overbrace{a^m|\phi'\rangle} = (\phi^*)^n(\phi')^m\langle\phi|\phi'\rangle = (\phi^*)^n(\phi')^m e^{\phi^*\phi'}$$

$\Rightarrow \langle\phi| : A(a^\dagger, a) : |\phi'\rangle = e^{\phi^*\phi} A(\phi^*, \phi')$

(e) Let $I \equiv \int \frac{d\phi\, d\phi^*}{2\pi i} e^{-\phi^*\phi}|\phi\rangle\langle\phi|$ and look what happens when I acts on an arbitrary vector $|\phi'\rangle$:

$$\begin{aligned} I|\phi'\rangle &= \int \frac{d\phi\, d\phi^*}{2\pi i} e^{-\phi^*\phi}|\phi\rangle\langle\phi|\phi'\rangle \\ &= \int \frac{d\phi\, d\phi^*}{2\pi i} e^{-\phi^*\phi}|\phi\rangle\, e^{\phi^*\phi'} \\ &= \int \frac{d\phi\, d\phi^*}{2\pi i} e^{\phi^*(\phi'-\phi)}|\phi\rangle \\ &= \int \frac{d\phi}{2\pi i}\, 2\pi i\, \delta(\phi'-\phi)|\phi\rangle \\ &= |\phi'\rangle \end{aligned}$$

So I has the same effect as the identity operator $\mathbb{1}$.

Alternatively, as the same as in all Gaussian type integral, you can convert to polar coordinates and do the integral. (Use $\phi = re^{i\theta}, \phi^* = re^{-i\theta}$).

Note that *coherent state* in this context is nothing but a displaced vacuum state expressed in unshifted energy eigenstates. It also satisfies the minimal uncertainty relation.

2. Define a *squeezed state* to be a state of the form

$$|\alpha, \beta, \gamma\rangle = e^{\alpha+\beta a^\dagger+\gamma(a^\dagger)^2}|0\rangle \tag{1}$$

in the single harmonic oscillator Hilbert space

(a) Compute the norm $\langle\alpha, \beta, \gamma|\alpha, \beta, \gamma\rangle$ in the special case $\beta = 0$. What is the condition needed for this norm to be finite? Extra credit: can you generalize your result to $\beta \neq 0$?

(b) Show that the position basis state $|x'\rangle$ can be written in the form (1), and find the associated values $\alpha(x'), \beta(x'), \gamma(x')$. Does your expression for $|x'\rangle$ give a state of finite norm in the Hilbert space?

Answer:

(a)

$$\| \ \|^2 = e^{\alpha^*+\alpha}\langle 0|e^{\gamma_1^* a^2} e^{\gamma_2 (a^\dagger)^2}|0\rangle = e^{\alpha^*+\alpha}\sum_{m,n}\langle 0|(a^2)^n \frac{(\gamma_1^*)^n}{n!}\frac{(\gamma_2)^m}{n!}((a^\dagger)^2)^m|0\rangle$$

$$\langle 0|(a^2)^n((a^\dagger)^2)^m|0\rangle = \sqrt{(2n)!}\sqrt{(2m)!}\ \delta_{n,m}$$

$\Rightarrow \| \ \|^2 = e^{\alpha^*+\alpha}\langle 0|\sum_n \frac{(\gamma_1^*\gamma_2)^n}{n!n!}(2n)!|0\rangle$

Several methods to get the sum sandwiched:

– you recognize it's the binomial expansion of $\frac{1}{\sqrt{1-4\gamma_1^*\gamma_2}}$

– Put in Mathematica:
`Sum[(añ (2 n)!)/(n! n!),n,0,Infinity]`, and it gives you the same answer.

– Another frequently used trick (generating funtion): $g(z) \equiv \sum_n \frac{z^n(2n)!}{n!\,n!}$, differentiate w.r.t z, we get $g'(z) = 2g(z) + 4zg'(z)$. Using the boundary condition $g(z=0) = 1$, we get $g(z) = \frac{1}{\sqrt{1-4z}}$.

For $\beta = 0$, we need $|\gamma| < 1/2$ so the norm is finite.

For $\beta \neq 0$, first we need a commutator similar to the one mentioned in 5(b): $[e^{\gamma^* a^2}, a^\dagger] = 2\gamma^* a e^{\gamma^* a^2}$ and $[a, e^{\gamma(a^\dagger)^2}] = 2\gamma a^\dagger e^{\gamma(a^\dagger)^2}$.

We also need to know a couple of things to help us not lost in the symbol jungle:

(a) $a^\dagger$ is free to move back and forth in the crowds of its fellow. In our case, $a^\dagger$, $e^{\beta a^\dagger}$, and $e^{\gamma(a^\dagger)^2}$ can be interchanged. The same situation for a.

(b) The solution for the following ODE:

$$\frac{d\,y}{d\,x} = (ax + b)y$$

is

$$y = \text{constant} \times e^{bx + \frac{a}{2}x^2}$$

Then

$$\begin{aligned} \| \, \|^2 &= \langle \alpha, \beta, \gamma | \alpha, \beta, \gamma \rangle \\ &= e^{\alpha^* + \alpha} \langle 0 | e^{\beta^* a} e^{\gamma^* a^2} e^{\beta a^\dagger} e^{\gamma(a^\dagger)^2} | 0 \rangle \\ &\equiv e^{\alpha^* + \alpha} F(\beta, \beta^*) \end{aligned}$$

Now again is the same old trick, we differentiate $F(\beta, \beta^*)$ to get some relation:

$$\begin{aligned} \frac{\partial F}{\partial \beta^*} &= \langle 0 | e^{\beta^* a} e^{\gamma^* a^2} a e^{\beta a^\dagger} e^{\gamma(a^\dagger)^2} | 0 \rangle \\ &= \langle 0 | e^{\beta^* a} e^{\gamma^* a^2} \underbrace{a e^{\gamma(a^\dagger)^2}}_{e^{\gamma(a^\dagger)^2}(a + 2\gamma a^\dagger)} \underbrace{e^{\beta a^\dagger} | 0 \rangle}_{|\beta\rangle} \\ &= \beta F + 2\gamma \underbrace{\langle 0 | e^{\beta^* a}}_{\langle \beta |} \underbrace{e^{\gamma^* a^2} a^\dagger}_{(a^\dagger + 2\gamma^* a) e^{\gamma^* a^2}} e^{\beta a^\dagger} e^{\gamma(a^\dagger)^2} | 0 \rangle \\ &= \beta F + 2\gamma (\beta^* F + 2\gamma^* \frac{\partial F}{\partial \beta^*}) \end{aligned}$$

$$\Rightarrow \frac{\partial F}{\partial \beta^*} = \frac{\beta + 2\gamma\beta^*}{1 - 4|\gamma|^2} F$$

$\frac{\partial F}{\partial \beta}$ is conjugate to the above.

Now, let $a = \frac{2\gamma}{1-4|\gamma|^2}$, $b = \frac{\beta}{1-4|\gamma|^2}$,

$$\Rightarrow F(\beta, \beta^*) = \text{constant} \times e^{\frac{|\beta|^2 + \gamma(\beta^*)^2}{1-4|\gamma|^2}}$$

We should put one more term in the exponent which comes from $\frac{\partial F}{\partial \beta}$: $\frac{\gamma^* \beta^2}{1-4|\gamma|^2}$. The constant is determined from the fact that this solution should be the same as the one we obtained earlier when $\beta = 0$, and $\beta^* = 0$. So constant $= \frac{1}{\sqrt{1-4|\gamma|^2}}$.

Finally,

$$\boxed{F(\beta, \beta^*) = \frac{1}{\sqrt{1-4|\gamma|^2}} e^{\frac{|\beta|^2 + \gamma(\beta^*)^2 + \gamma^* \beta^2}{1-4|\gamma|^2}}}$$

and the normalization condition is the same:

$$\boxed{|\gamma| < 1/2}$$

.

(b) Use almost the same trick as part(a). We want to find β and γ for state $|x'\rangle$ where $x|x'\rangle = x'|x'\rangle$. Let

$$|x'\rangle = |\beta, \gamma\rangle = e^{\beta a^\dagger + \gamma (a^\dagger)^2} |0\rangle$$

Using

$$x = \frac{1}{\sqrt{2}}(a + a^\dagger)$$

Then again

$$\underbrace{a e^{\gamma (a^\dagger)^2}}_{e^{\gamma (a^\dagger)^2}(a + 2\gamma a^\dagger)} \underbrace{e^{\beta a^\dagger}|0\rangle}_{|\beta\rangle} = \beta |\beta, \gamma\rangle + 2\gamma a^\dagger |\beta, \gamma\rangle$$

$$\Rightarrow \frac{1}{\sqrt{2}}(a + a^\dagger)|\beta, \gamma\rangle = \frac{1}{\sqrt{2}} \left[(\beta + 2\gamma a^\dagger + a^\dagger)\right] |\beta, \gamma\rangle$$

We then make it equal to $x'|\alpha, \beta, \gamma\rangle$ by choosing

$$\boxed{\beta = \sqrt{2}x', \text{ and } \gamma = -\tfrac{1}{2}}$$

α is found by normalization:

$$\langle 0|x'\rangle = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{1}{2}x'^2} = \langle 0|\alpha, \beta, \gamma\rangle = e^\alpha \times \underbrace{\langle 0|\beta, \gamma\rangle}_{1 \text{ by expand the exponents}}$$

We see that $|\gamma| = 1/2$, so it's not normalizable. This is reasonable, since the state itself is not normalizable in $x-$space, and this wouldn't change by changing to another bases.

Alternatively, we can do this in a more elementary way as follows:

$$\begin{aligned} |\alpha, \beta, \gamma\rangle &= e^\alpha e^{\beta a^\dagger} e^{\gamma (a^\dagger)^2} |0\rangle \\ &= e^\alpha \sum_{n,n'} \frac{(\beta a^\dagger)^n}{n!} \frac{(\gamma (a^\dagger)^2)^{n'}}{n'!} |0\rangle \\ &\equiv |x'\rangle \end{aligned}$$

Note

$$\phi_n(x) \equiv \langle x|n\rangle = \left(\frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x^2}{2}}\right) \frac{1}{\sqrt{2^n n!}} H_n(x)$$

where $H_n(x)$ is Hermite function, and $H_0(x) = 1$, $H_1(x) = 2x$, $H_2(x) = 4x^2 - 2$.
By projecting $|\alpha, \beta, \gamma\rangle$ to $|0\rangle$, $|1\rangle$, and $|2\rangle$ respectively, we can obtain α, β, and γ!

(i)

$$\langle 0|x'\rangle = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x'^2}{2}} H_0(x') = e^{\alpha} \quad \text{only } n = 0 = n' \text{ has contribution}$$

(ii)

$$\langle 1|x'\rangle = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x'^2}{2}} \frac{1}{\sqrt{2}} H_1(x') = e^{\alpha}\beta \quad \text{only } n = 1, n' = 0 \text{ has contribution}$$

(iii)

$$\langle 2|x'\rangle = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x'^2}{2}} \frac{1}{\sqrt{2^2 2!}} H_2(x') = e^{\alpha}\left(\frac{\beta^2}{2} + \gamma\right) \quad \times \underbrace{\sqrt{2}}_{\langle 2|(a^\dagger)^2|0\rangle = \sqrt{2}}$$

only $n = 0, n' = 1$, and $n = 2, n' = 0$ has contribution

From (i) $\Rightarrow e^{\alpha} = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x'^2}{2}}$.
From (ii) $\Rightarrow \beta = \frac{1}{\sqrt{2}} H_1(x') = \sqrt{2}x'$.
From (iii) $\Rightarrow (\frac{\beta^2}{2} + \gamma)\sqrt{2} = \frac{1}{\sqrt{2^2 2!}} H_2(x') = \frac{1}{\sqrt{8}}(4x'^2 - 2) \Rightarrow \gamma = -\frac{1}{2}$.
The dimensional expression is

$$e^{\alpha} = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{\hbar}\frac{x'^2}{2}}$$

$$\beta = \sqrt{2}x'\sqrt{\frac{m\omega}{\hbar}}$$

$$\gamma = -\frac{1}{2} \quad \text{unchange!}$$

3. For each part of this problem you are asked to find an approximation to the energies of one or more of the lowest-lying quantum states for a particular potential. You may use any approximation technique you wish to determine the energy eigenvalues. You may use a computer if you wish, or you can work by hand. (Note that a good way to check your answers yourself is to try using several different methods!) Please include a sketch or graph of the eigenfunctions in each case. In all parts you should use units with $\hbar = m = 1$.

(a) Find the ground state and first excited state energies for a particle in the 1D potential

$$V(x) = \frac{1}{4}x^4 \,.$$

(b) Find the ground state and first excited state energies for a particle in the 1D potential

$$V(x) = -\frac{1}{2}x^2 + \frac{1}{24}x^4 \,.$$

(c) Find the ground state energy for a pair of particles in the harmonic oscillator potential $V(x) = x^2/2$. The interaction energy between the particles is given by $-\sqrt{2}|x-y|$, where x, y are the positions of the two particles. You may assume that these particles are fermions, so that $\psi(x,y) = -\psi(y,x)$. Note that the Hamiltonian for this system is equivalent to that of a single particle moving in two dimensions x, y in the potential

$$W(x,y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 - \sqrt{2}|x-y|\,.$$

(d) (Extra credit, optional): Find the ground state energy for a particle in the 2D potential

$$V(x,y) = \frac{1}{4}x^4 + \frac{1}{6}y^6 + 2xy\,.$$

Several different methods are detailed for Part(a).

(a) $V(x) = \frac{1}{4}x^4$

(i) Shooting method.
The following codes is specialized for Mathematica, but the spirit is the same for other programming languages.

First the Hamiltonian is defined:

$$\boxed{\text{hamiltonian}[V\_]@\psi\_ := -\frac{\hbar^2}{2m}\partial_{x,x}\psi + V\psi}$$

Here the function `hamiltonian` is written as hamiltonian$[V_]@\psi_$ rather than hamiltonian$[V_, \psi_]$. Both of them are the same in Mathematica, but conceptually, we think the potential V is a part of the Hamiltonian, and then the Hamiltonian operates on the wave function ψ.

Then is the Schrödinger equation

$$\boxed{\text{schroedingerD}[V\_]@\psi\_ := \text{hamiltonian}[V]@\psi - \text{Energy}\psi}$$

Now we can solve for the ground state:

$$\begin{aligned}&\text{solGround}\\ &= \text{NDSolve}[\{\text{schroedingerD}\left[\frac{1}{x}x^4\right]@\psi[x] == 0, \psi[0] == 1, \psi'[0] == 0\}\\ &\quad /.\{\hbar \to 1, m \to 1, \text{Energy} \to 0.4\}, \psi[x], \{x, 0, 6.1\}, \text{MaxSteps} \to 4000];\end{aligned}$$

The option `MaxSteps` specifies the maximum number of steps that `NDSolve` will ever take in attempting to find a solution. The default value is enough for our problem, here it is explicitly typed out, so you know what to change when you encounter problem for complicated potential, or for larger range of coordinate.

We know that for this symmetric potential, the ground state wave function has slope 0 at $x = 0$. The wave function can have any value at $x = 0$ since we haven't normalized it. Here we put it to be 1.

These three lines of codes are all we need. Now we guess a reasonable energy: 0.4 (for a potential $\frac{1}{4}x^2$, the ground state energy is $\frac{1}{2}\hbar\omega = 0.35$, so we know our target is a bit higher than 0.35).

From the command

$$\text{Plot}[\psi[x]/.\text{solGround}, \{x, 0, 6.1\}, \text{PlotRange} \to \{-2, 2\}, \text{AxesLabel} \to \{\text{“}x\text{”}, \text{“}\psi(x)\text{”}\}]$$

You should see a picture like this

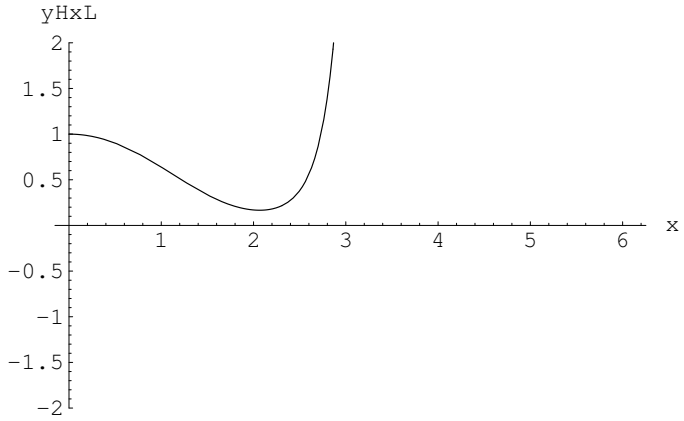

Figure 1: Lower energy

while for Energy= 0.43, you see a picture like this

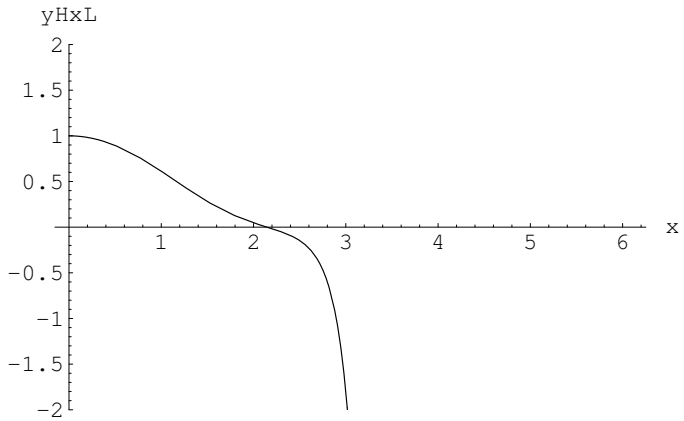

Figure 2: Higher energy

Here is an elementary explanation why Fig. 1 curve has *lower* energy than Fig. 2: Given a curve with a node (crossing with $x-$axis) like Fig. 2, we can always flip the negative

part, and then smooth the kink. The smoothed part has lower (negative) kinetic energy ($\propto -\frac{\partial^2}{\partial x^2} = (-)(+) < 0$), while ψ around that neighborhood is not increased too much, so the potential energy doesn't increase very much either.

Repeating this procedure, the lower and upper limit is narrowing down. You can automate this, although for this particular problem, human intervening (with a cup of coffee at hand) is fastest.

The answer is
$\boxed{0.420803158325285003 < \text{Ground State Energy} < 0.420803158325285004}$.

For first excited state energy, we use the initial condition $\psi[0] == 0$, and $\psi'[0] == 1$, and get
$\boxed{1.50789828279577148301008 < \text{First Excited} < 1.50789828279577148301009}$

(ii) Variational method.
The "variational method" takes several slightly different context. Usually, a trial wave function with several adjustable parameters is guessed. Then we minimize the energy to get an upper bound of the energy. For our problem, a good initial guess is $\psi(x) = e^{-ax^2}$, we then minimize $\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$ and obtain $a = \sqrt[3]{\frac{3}{16}}$, and get $E_0 \simeq 0.429268$, which of course we wouldn't expect very close to the exact answer. You can also use more complicated trial wave function $\psi(x) = e^{f(x)}$, where $f(x)$ is a polynomial in x, and the coefficients are treated as adjustable parameters. Notice that (1) the calculation becomes tedious, (2) for a general $f(x) = -ax^2 - bx^3 - cx^4$, say, even though this trial wave function doesn't have the right symmetry, $\psi(-x) \neq \psi(x)$, we can still get lower energy than using $\psi(x) = e^{-ax^2}$, which has the right symmetry. (3) When you expand $\psi(x) = e^{-ax^2}$ in SHO's basis, it is a linear combination for *all* basis.

On the other hand, we can restrict the dimension of Hilbert space to be finite, say the first few SHO's eigenvectors $|n\rangle$, and form an approximated Hamiltonian matrix with matrix element: $\langle m|H|n\rangle$ and calculate the eigenvalues of this approximated matrix. The eigenvectors thus formed is the linear superposition of these finite SHO eigenvectors and minimize the energy.

If the potential is like x^k, then all we need is the matrix element $\langle m|p^k|n\rangle$ ($k = 2$ for our case), and $\langle m|x^k|n\rangle$ (note recursion is used in the following codes, since $\langle m|x^k|n\rangle = \sum_j \langle m|x|j\rangle\langle j|x^{k-1}|n\rangle$, but only $j = m-1, m, m+1$ makes contribution. `ME` means matrix element):

```
xME[m_, n_, k_] :=
   xME[m, n, k] =
    If[k == 1, If[Abs[m - n] == 1, Sqrt[Max[m, n]/2], 0],
     Sum[xME[m, j, 1] xME[j, n, k - 1], {j, m - 1, m + 1}]];

pME[m_, n_, k_] :=
```

```
pME[m, n, k] =
 If[k == 1, If[Abs[m - n] == 1, I (m - n) Sqrt[Max[m, n]/2], 0],
  Sum[pME[m, j, 1] pME[j, n, k - 1], {j, m - 1, m + 1}]];

hamiltonianME[1, max_] :=
  Table[pME[m, n, 2]/2 + xME[m, n, 4]/4, {m, 0, max}, {n, 0, max}];

ground[i_,max_]:=Take[Sort[Eigenvalues[N[hamiltonianME[i,max]]]],2];
```

then `ground[1, 11]` gives you `0.420825,1.50793`. Notice that the ground state energy approaches the exact value faster than the first excited energy.

(b) The potential looks like

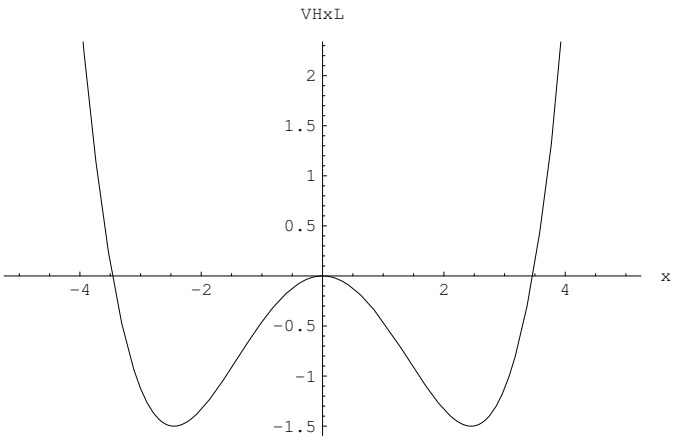

Figure 3: $V(x) = -\frac{1}{2}x^2 + \frac{1}{24}x^4$

and the energy is

$$\boxed{-0.85562342156 < \text{Ground State Energy} < -0.85562342155}$$

and

$$\boxed{-0.8298890522702 < \text{First Excited} < -0.8298890522701}$$

We see the first excited state energy is very close to the ground state energy. This is anticipated, since classically there are two degenerate ground states; while due to quantum mechanical tunnelling, the degeneracy is removed. The energy splitting is determined by the barrier separated the two wells. The ground state is symmetric, and the first excited state antisymmetric.

(c) As hinted by the problem, this part is equivalent to finding the first excited energy in the 2D potential

$$W(x, y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 - \sqrt{2}\,|x - y|$$

This particular form makes direct application of the variational method impossible. (We don't know what $|a + a^\dagger|$ is.)

However, this potential is separable:

$$u \equiv \frac{1}{\sqrt{2}}(x+y), \quad v \equiv \frac{1}{\sqrt{2}}(x-y)$$

and the potential becomes

$$W(u,v) = \frac{1}{2}u^2 + \frac{1}{2}v^2 - 2\,|v|$$

The $u-$part is a SHO, with $E_0^u = \frac{1}{2}$, $E_1^u = \frac{3}{2}$.

The $v-$part looks like

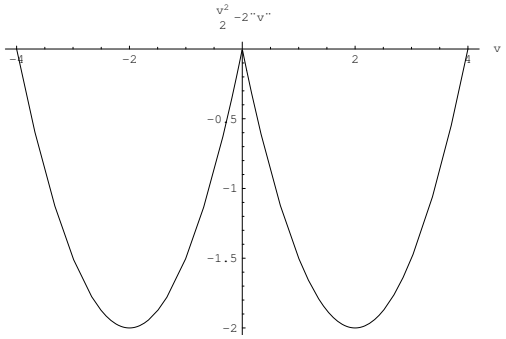

Figure 4: $\frac{1}{2}v^2 - 2\,|v|$

Using the shooting method described in Part(a), we get $E_0^v = -1.524$, $E_1^v = -1.482$. The energy levels for the *2D* problem therefore is:
`-1.024,-0.982,-0.024,0.018`.

So the ground state energy for the original two fermion in 1D is: $\boxed{-0.982}$.

(d) $V(x) = \frac{1}{4}x^4 + \frac{1}{5}x^6 + 2xy$.

The variational method is used for this part.

The most naive and direct choice of basis is

$$|i,j\rangle \equiv |i\rangle \otimes |j\rangle$$

where $|i\rangle$, and $|j\rangle$ are energy eigen basis of SHO. If we use s states for each, then the dimension of the (restricted) Hilbert space is $s \times s = s^2$. That is, $|0,0\rangle \equiv |\mathbf{1}\rangle, |0,1\rangle \equiv |\mathbf{2}\rangle, \ldots, |s,s\rangle \equiv |\mathbf{s^2}\rangle$. The Hamiltonian is thus a $s^2 \times s^2$ matrix.

Now, we do a reverse thinking: given $|\mathbf{n}\rangle$, what is $|i\rangle$, and $|j\rangle$ such that $|i\rangle \otimes |j\rangle = |\mathbf{n}\rangle$? After a few seconds' thinking, you realize $\mathbf{n} = i \times s + (j+1)$. So i is the `Quotient`, and $j+1$ is the `Reminder`. That is,

```
i=Quotient[n,s], j=Mod[n,s]-1
```

If $|\mathbf{n}\rangle = |i\rangle \otimes |j\rangle$, $|\mathbf{m}\rangle = |i'\rangle \otimes |j'\rangle$, then we get

$$\langle \mathbf{m}|H|\mathbf{n}\rangle = \langle i'|\frac{p_x^2}{2m}|i\rangle\delta_{j,j'} + \langle j'|\frac{p_y^2}{2m}|j\rangle\delta_{i,i'} + \frac{1}{4}\langle i'|x^4|i\rangle\delta_{j,j'} + \frac{1}{6}\langle j'|y^6|j\rangle\delta_{i,i'} + 2\langle i'|x|i\rangle\langle j'|y|j\rangle$$

Now we can write the code as follows:

```
<<DiscreteMath‘KroneckerDelta‘

hamiltonianME[2, s_]:= Table[
 KroneckerDelta[Mod[n,s]-Mod[m,s]] (pME[Quotient[m,s], Quotient[n,s],
2]/2)
 + KroneckerDelta[Quotient[n,s]-Quotient[m,s]] (pME[Mod[m,s]-1,
Mod[n,s]-1, 2]/2)
 + KroneckerDelta[Mod[n,s]-Mod[m,s]]
(xME[Quotient[m,s],Quotient[n,s],4]/4)
 + KroneckerDelta[Quotient[n,s]-Quotient[m,s]] (xME[Mod[m,s]-1,
Mod[n,s]-1,6]/6)
 + 2 xME[Quotient[m,s], Quotient[n,s],1] xME[Mod[m,s]-1, Mod[n,s]-1,1],
        {m,1,s^2},{n,1,s^2}]
```

Then the command `ground[2,30]` gives you `0.387339, 0.637318`, in only a few minutes. You might ask, why do we need such many states (in our case, 30×30) to achieve the accuracy? The answer of course is that our trial wavefunciton, the eigenfunctions for SHO, are not as good as in the previous part. The potential is not always positive, and has four (symmetric) dips: $V(\pm(2^{2/7}, -2^{3/7})) = -1.73863$. If you construct trial wavefunctions such that they have more weight around those 4 points, faster convergence can be achieved. Another possibility is that you notice $\langle \mathbf{m}|x^k|\mathbf{n}\rangle \sim \mathcal{O}(\sqrt{n^k})$ if it is not 0. This implies you should use more number of $y-$basis than $x-$basis. So instead of 30×30, use 23×40 basis. Since the codes we outlined above is very efficient, the time you spend on searching for more efficient basis, or best combination of number of basis, might greatly more than the naive and direct one ... but it is still very interesting to explore by yourself.