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Course: **8.321 - Quantum Theory I**
Problem set: **#5**

1. Coherent states

(a)

$$\left|\phi\right\rangle = e^{\phi a^\dagger}\left|0\right\rangle = \sum_{n=0}^{\infty}\frac{\phi^n (a^\dagger)^n}{n!}\left|0\right\rangle = \sum_{n=0}^{\infty}\frac{\phi^n}{n!}\sqrt{n!}\left|n\right\rangle = \sum_{n=0}^{\infty}\frac{\phi^n}{\sqrt{n!}}\left|n\right\rangle.$$

(b)

$$a\left|\phi\right\rangle = \sum_{n=0}^{\infty}\frac{\phi^n}{\sqrt{n!}}a\left|n\right\rangle = \sum_{n=0}^{\infty}\frac{\phi^n}{\sqrt{n!}}\sqrt{n}\left|n-1\right\rangle = \phi\sum_{n-1=0}^{\infty}\frac{\phi^{n-1}}{\sqrt{(n-1)!}}\left|n-1\right\rangle = \phi\left|\phi\right\rangle.$$

(c)

$$\left\langle\phi|\phi'\right\rangle = \sum_{m=0}^{\infty}\frac{(\phi^*)^m}{\sqrt{m!}}\sum_{n=0}^{\infty}\frac{\phi'^n}{\sqrt{n!}}\left\langle m|n\right\rangle = \sum_{n=0}^{\infty}\frac{(\phi^*\phi')^n}{n!} = e^{\phi^*\phi'}.$$

(d)

$$\left\langle\phi\right| : A(a^\dagger, a) : \left|\phi'\right\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}C(m,n)\left\langle\phi\right|(a^\dagger)^m a^n\left|\phi'\right\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}C(m,n)(\phi^*)^m\phi'^n\left\langle\phi|\phi'\right\rangle = e^{\phi^*\phi'}A(\phi^*,\phi')$$

(e)

$$\frac{1}{2\pi i}\int d\phi^* d\phi e^{-\phi^*\phi}\left|\phi\middle\rangle\middle\langle\phi\right| = \frac{1}{2\pi i}\sum_{n,m}^{\infty}\frac{\left|m\right\rangle\left\langle n\right|}{\sqrt{m!n!}}\int d\phi^* d\phi(\phi^*)^n\phi^m e^{-\phi^*\phi}$$

In polar coordinates, $\phi = re^{i\theta}$, and $\int d\phi^* d\phi = 2i\int r\,drd\theta$ (where we treat $\phi = x+iy$ and $\phi^* = x-iy$ as independent variables to get $d\phi^* d\phi = 2idxdy$). With this,

$$\begin{aligned}\frac{1}{2\pi i}\sum_{n,m}^{\infty}\frac{\left|m\right\rangle\left\langle n\right|}{\sqrt{m!n!}}\int d\phi^* d\phi e^{-\phi^*\phi}\left|\phi\middle\rangle\middle\langle\phi\right| &= \frac{2i}{2\pi i}\sum_{n,m}^{\infty}\frac{\left|m\right\rangle\left\langle n\right|}{\sqrt{m!n!}}\int_0^{2\pi}d\theta e^{i(m-n)\theta}\int_0^{\infty}dr r^{m+n+1}e^{-r^2}\\ &= \frac{2i}{2\pi i}\sum_{n,m}^{\infty}\frac{\left|m\right\rangle\left\langle n\right|}{\sqrt{m!n!}}2\pi\delta_{mn}\frac{1}{2}\Gamma\left(\frac{2+m+n}{2}\right)\\ &= \frac{2i}{2i}\sum_{n=0}^{\infty}\frac{\left|n\right\rangle\left\langle n\right|}{n!}\Gamma(n+1)\\ &= \frac{2i}{2i}\sum_{n=0}^{\infty}\frac{\left|n\right\rangle\left\langle n\right|}{n!}n!\\ &= \mathbb{I}.\end{aligned}$$

2. Squeezed states

(a) When $\beta = 0$ we have

$$\langle \alpha, 0, \gamma | \alpha, 0, \gamma \rangle = e^{\alpha^* \alpha} \langle 0 | \left(e^{\gamma (a^\dagger)^2} \right)^\dagger e^{\gamma (a^\dagger)^2} |0\rangle$$
$$= e^{\alpha^* \alpha} \langle 0 | e^{\gamma^* a^2} e^{\gamma (a^\dagger)^2} |0\rangle$$

Let's calculate $e^{\gamma (a^\dagger)^2} |0\rangle$:

$$e^{\gamma (a^\dagger)^2} |0\rangle = \sum_{n=0}^{\infty} \frac{\gamma^n (a^\dagger)^n (a^\dagger)^n}{n!} |0\rangle$$
$$= \sum_{n=0}^{\infty} \frac{\gamma^n}{\sqrt{n!}} (a^\dagger)^n |n\rangle$$
$$= \sum_{n=0}^{\infty} \frac{\gamma^n}{\sqrt{n!}} \sqrt{\frac{(2n)!}{n!}} |2n\rangle$$
$$\sum_{n=0}^{\infty} \frac{\gamma^n}{n!} \sqrt{(2n)!} |2n\rangle .$$

With this,

$$\left\langle \alpha, 0, \beta \middle| \alpha, 0, \beta \right\rangle = e^{\alpha^* \alpha} \sum_{n,m}^{\infty} \frac{(\gamma^*)^n \gamma^m}{n! m!} \sqrt{(2n)!(2m)!} \delta_{mn} = e^{\alpha^* \alpha} \sum_{n=0}^{\infty} \frac{|\gamma|^{2n}}{(n!)^2} (2n)!$$

In order for this norm to converge, the series must satisfy the ratio test:

$$1 > e^{|\alpha|^2} \lim_{n \to \infty} \frac{|\gamma|^{2(n+1)} (2(n+1))!/((n+1)!)^2}{|\gamma|^{2n} (2n)!/(n!)^2} = \lim_{n \to \infty} e^{|\alpha|^2} |\gamma|^2 \frac{(2n+1)(2n+2)}{(n+1)(n+1)} = 4 e^{|\alpha|^2} |\gamma|^2 \implies \boxed{e^{|\alpha|^2} |\gamma|^2 < 1/4}$$

Extend this result for $\beta \neq 0$? Complete the square? Not sure how to do this.

(b) We claim that

$$\boxed{|x'\rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} x'^2 \right) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger - \frac{1}{2} (a^\dagger)^2 \right) |0\rangle}$$

from which we read off the coefficients:

$$\gamma = -\frac{1}{2}, \qquad \beta = \sqrt{\frac{2m\omega}{\hbar}} x', \qquad \alpha = -\frac{m\omega}{2\hbar} x'^2 + \frac{1}{4} \ln\left(\frac{m\omega}{\pi\hbar} \right).$$

Now we prove that the boxed equation is true. To this end, we check that the normalization is correct and that the the equation $\hat{x} |x'\rangle = x' |x'\rangle$ is satisfied.

$$\hat{x} |x'\rangle = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) |x'\rangle$$
$$= \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} x'^2 \right) \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger - \frac{1}{2} (a^\dagger)^2 \right) |0\rangle$$
$$= \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} x'^2 \right) \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \exp\left(-\frac{1}{2} (a^\dagger)^2 \right) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger \right) |0\rangle$$

since things commute. This is rather complicated to deal with. However, we may insert the identity operator I defined by

$$I = \exp\left(-\frac{1}{2}(a^\dagger)^2\right) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger\right) \exp\left(-\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger\right) \exp\left(\frac{1}{2}(a^\dagger)^2\right)$$

to the left and observe that

$$\begin{aligned}
\exp\left(\frac{1}{2}(a^\dagger)^2\right)(a + a^\dagger)\exp\left(-\frac{1}{2}(a^\dagger)^2\right) &= \exp\left(\frac{1}{2}(a^\dagger)^2\right) a \exp\left(-\frac{1}{2}(a^\dagger)^2\right) + a^\dagger \\
&= a + \frac{1}{2}[a^\dagger a^\dagger, a] + a^\dagger \\
&= a + \frac{1}{2}(a^\dagger[a^\dagger, a] + [a^\dagger, a]a^\dagger) + a^\dagger \\
&= a - a^\dagger + a^\dagger \\
&= a,
\end{aligned}$$

where we have used the identity for $e^A B e^{-A}$ from Pset 1 and the fact that $a^\dagger$ commutes with itself. Next, we find (using the same identity)

$$\begin{aligned}
\exp\left(-\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger\right) a \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger\right) &= a - \sqrt{\frac{2m\omega}{\hbar}} x' [a^\dagger, a] \\
&= a + \sqrt{\frac{2m\omega}{\hbar}} x'.
\end{aligned}$$

Since $a\,|0\rangle = 0$, we have

$$\begin{aligned}
\hat{x}\,|x'\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x'^2\right) \cancel{\sqrt{\frac{\hbar}{2m\omega}}} \exp\left(-\frac{1}{2}(a^\dagger)^2\right) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger\right) \cancel{\sqrt{\frac{2m\omega}{\hbar}}}\, x'\,|0\rangle \\
&= x' \left\{ \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x'^2\right) \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x' a^\dagger - \frac{1}{2}(a^\dagger)^2\right)|0\rangle \right\} \\
&= x'\,|x'\rangle \qquad \checkmark
\end{aligned}$$

The normalization is obtained by finding $\langle 0|x'\rangle$. Suppose that it is N, then

$$\langle 0|x'\rangle = N\,\langle 0| \exp\left(\sqrt{\frac{2m\omega}{\hbar}} x a^\dagger - \frac{1}{2}(a^\dagger)^2\right)|0\rangle = N\,\langle 0|0\rangle = N \implies N = \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x'^2\right).$$

With this we're done.

To see if $\langle x'|x'\rangle$ is bounded or not, we may look at $\langle x = 0|x = 0\rangle$ where from Part (c) we require that $e^{|\alpha|^2}|\gamma|^2 < 1$. Notice that $e^{|\alpha|^2} \geq 1$ for all α, and so the norm is finite only if $\gamma^2 < 1/4$. However, in this case we have $\gamma = -1/2 \implies \gamma^2 = 1/4$. We therefore conclude that $\langle x'|x'\rangle$ is infinite, as expected.

3. Low-lying states

(a) Ground and first excited energy for particle in the potential:

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

We may solve this problem using two different techniques.

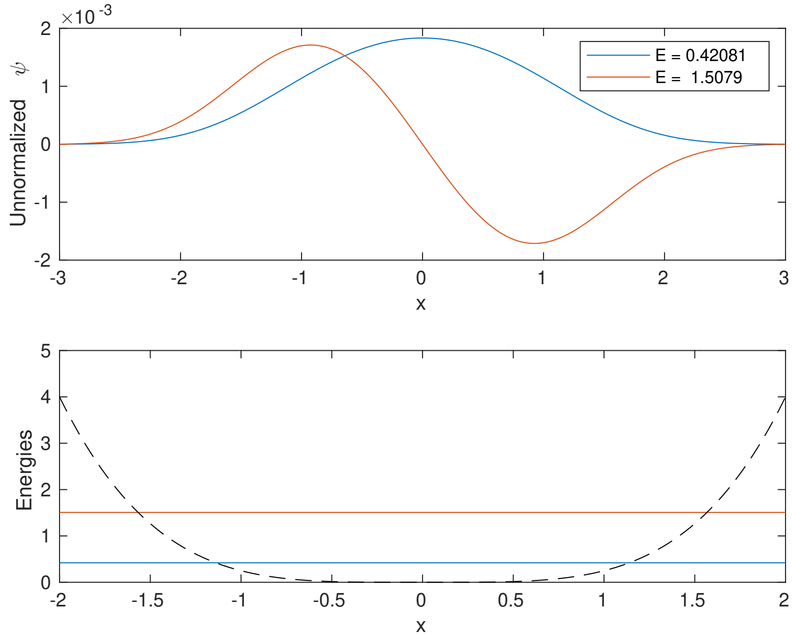
Finite-difference method: The Hamiltonian has the form

$$\mathcal{H} = -\frac{1}{2\Delta x^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & & \\ & & 1 & \ddots & 1 \\ & & & & -2 \end{pmatrix} + \frac{x^4}{4}\mathbb{I}.$$

After solving in MATLAB, I found that the two lowest energies are

$$\boxed{E_0 \approx 0.421} \qquad \boxed{E_1 \approx 1.508}$$

Here is the graphical solution.



MATLAB code:

```
%%% Huan Q. Bui

N = 1e6; % No. of points.
hbar = 1;
m = 1;
x_start = -3;
x_end = 3;
x = linspace(x_start, x_end, N).'; % Generate column vector with N
dx = x(2) - x(1); % Coordinate step

% Three-point finite-difference representation of Laplacian
e = ones(N,1); % a column of ones
Lap = spdiags([e -2*e e],[-1 0 1],N,N) / (dx^2);

% potential
U = x.^4/4;
% Total Hamiltonian.
H = -(1/2)*(hbar^2/m)*Lap + spdiags(U,0,N,N); % 0 indicates main diagonal

% Find lowest nmodes eigenvectors and eigenvalues of sparse matrix.
nmodes = 2;
[V,E] = eigs(H,nmodes,'SM'); % find two smallest eigenvalues
[E,ind] = sort(diag(E)); % convert E to vector and sort low to high.
```

```
V = V(:,ind); % rearrange corresponding eigenvectors.

% Generate plot of lowest energy eigenvectors V(x) and U(x).
figure(1);
subplot(2,1,1)
plot(x, V);
xlabel('x');
ylabel('Unnormalized \psi');
xlim([x_start x_end]);
% Add legend showing Energy of plotted V(x).
legendLabels = [repmat('E = ',nmodes,1), num2str(E)];
legend(legendLabels)

subplot(2,1,2)
plot(x, (E(1))*ones(N,1),...
x, (E(2))*ones(N,1), x, U, '--k');
xlabel('x');
ylabel('Energies');
xlim([x_start/2 x_end/2]);
```

Variational method: Alternatively, we could choose our guess solution for the ground state to be

$$\psi_0(x,\alpha) = \Phi_0(x,\alpha)$$

where α is a parameter and $\Phi_0(x,\alpha)$ is the ground state of the harmonic oscillator parameterized by α and is given by

$$\Phi_0(x,\alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha x^2}{2}\right)$$

The Rayleight-Ritz is given by

$$E(\alpha) = \frac{\int \psi \mathcal{H} \psi \, dx}{\int \psi^2 \, dx} = \int \psi \mathcal{H} \psi \, dx = \frac{3+4a^3}{16a^2} \implies \frac{\partial E}{\partial \alpha} = -\frac{3}{8a^3} + \frac{1}{4} = 0 \iff \alpha = \left(\frac{3}{2}\right)^{1/3}$$

Upon checking this that $E(\alpha)$ obtains a minimum at $\alpha =$, we conclude that the ground state energy found using this naive variational method is

$$\boxed{E_0 = \frac{3+4(3/2)}{16(3/2)^{2/3}} \approx 0.429}$$

which is consistent with what we found before.

For the first excited state, we do the same thing except that we start from the first-excited wavefunction of the harmonic oscillator.

$$\psi(x,\alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\, x \exp\left(-\frac{\alpha x^2}{2}\right).$$

Repeating the same procedure we find

$$\boxed{E_1(\alpha) = \frac{3(5+4a^3)}{16a^2} \implies E_1 \approx \min E(\alpha) = 1.527}$$

which is again consistent with what we found by solving the SE numerically.

(b) Correction: instead of using `SM` in MATLAB which picks out the smallest amplitude eigenvalues we have to use `sr` which picks out the smallest real. The MATLAB code is now updated, so check the MATLAB code for the correct solution.

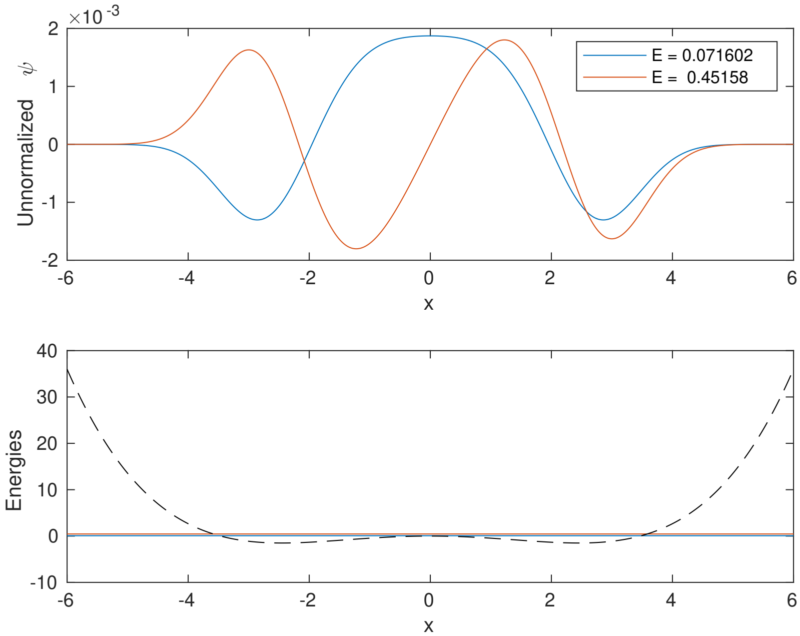
Ground and first excited energy for particle in the potential:

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

Finite-difference method: Using the same 1D SE solver as before, we find that

$$\boxed{E_0 \approx 0.072} \qquad \boxed{E_1 \approx 0.452}$$

Here is the graphical solution.



The MATLAB code is identical to the MATLAB code in Part (a), except that the potential energy $V(x)$ is modified:

```
% potential
U = -x.^2/2 + x.^4/24;
```

Shooting method: Searching for the ground state and first excited state energies via the shooting method we find with good accuracy:

$$\boxed{E_0 \approx 0.07160236} \qquad \boxed{E_1 \approx 0.45157662}$$

Mathematica code:

```
(*Double well potential*)
v[x_] := -x^2/2 + x^4/24;
xMax = 6;

(*ground state energy*)
energy = 0.07160236;
solution =
NDSolve[{psi''[x] == -2 (energy - v[x]) psi[x], psi[-xMax] == 0,
psi'[-xMax] == 0.001}, psi, {x, -xMax, xMax}];

Plot[psi[x] /. solution, {x, -xMax, xMax}]

(*First excited state energy*)
energy = 0.45157662;
solution =
NDSolve[{psi''[x] == -2 (energy - v[x]) psi[x], psi[-xMax] == 0,
psi'[-xMax] == 0.001}, psi, {x, -xMax, xMax}];

Plot[psi[x] /. solution, {x, -xMax, xMax}]
```

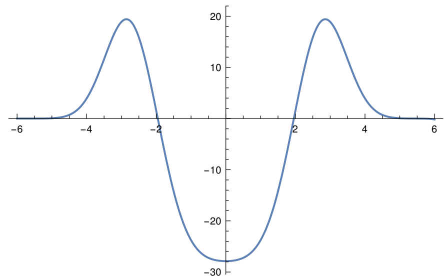


Figure 1: Ground state wavefunction

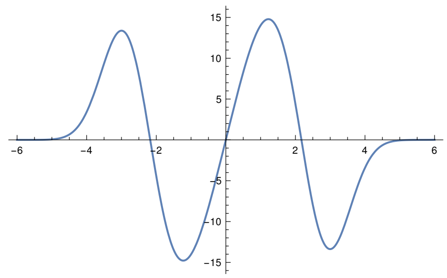


Figure 2: First excited state wavefunction

Shooting method output wavefunctions (up to overal phase factor compared to finite difference method):

(c) Correction: instead of using `SM` in MATLAB which picks out the smallest amplitude eigenvalues we have to use `sr` which picks out the smallest real. Update graphics shown below.

Ground state energy for particle in the potential:

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

where we require that $\psi(x,y) = -\psi(y,x)$.

Finite difference method: I'm solving this problem in MATLAB, using the method of finite difference. To do this, I referenced this page for a way to efficiently generate the 2D Laplacian operator. Once the Laplacian was setup, I had to test if my MATLAB code actually produces the correct energies for the usual 2D harmonic oscillator problem. And it did. Solving the 2D harmonic potential problem with $\omega = 1$ on a 100×100 grid where $x, y \in [-4, 4]$, I got the following energies for the lowest 4 eigenstates:

```
Lowest energies requested:
0.9996
1.9988
1.9988
2.9973
```

which are close to the correct values of $1, 2, 2, 3$ (as there is a two-fold degeneracy in the first excited state). With this I proceeded to solve the problem for the modified potential:

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

The caveat is that the lowest-energy solution to this problem is not what we want, since we also require that $\psi(x,y) = -\psi(y,x)$. This means that $\psi(x)$ must change sign under a reflection about the $y = x$ axis. To get to the correct solution, I had to go through the lowest-lying states and select the desired ψ with the lowest energy. The result is the state with energy

$$\boxed{E \approx 0.0320}$$

We also notice that the discarded solutions have negative energies.

```
Lowest energies requested:
-0.1229
-0.0127
0.0320
0.1291
```

The graphical solution is given below. wrong solution... this gotten by `SM` in MATLAB.

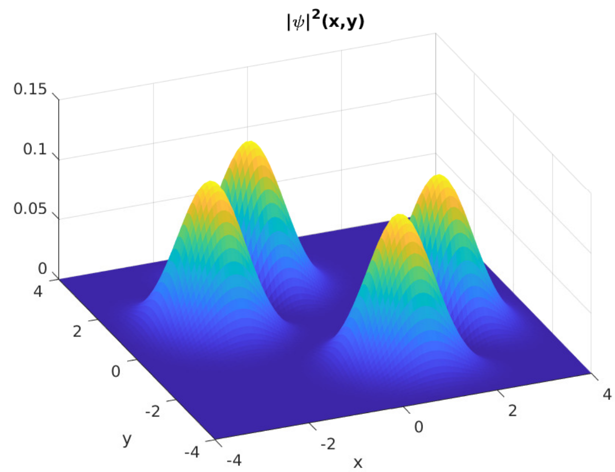


Figure 3: "Good" ground state density function

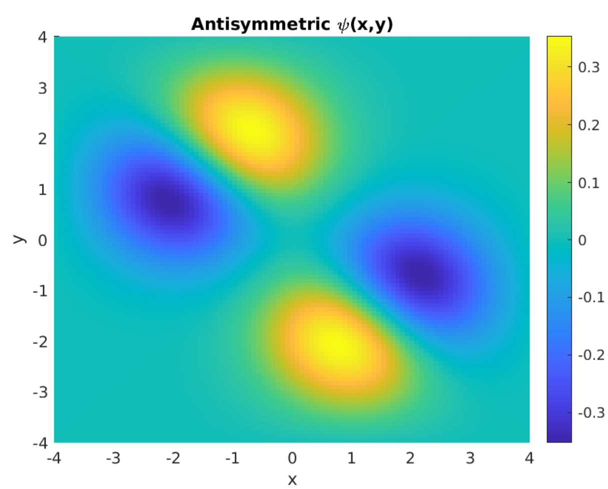


Figure 4: "Good" ground state wavefunction

Full MATLAB code:

```
hbar = 1;
m = 1;

N = 10^2;
L = 4;

x = linspace(-L,L,N);
y = linspace(-L,L,N);

dx= x(2) - x(1);
dy= y(2) - y(1);
```

```
%%% generate the 2D Laplacian operator quickly %%%
%%% source:
%%% https://www.mathworks.com/matlabcentral/fileexchange/69885-q_schrodinger2d_demo

Axy = ones(1,(N-1)*N);
DX2 = (-2)*diag(ones(1,N*N)) + (1)*diag(Axy,-N) + (1)*diag(Axy,N);

AA = ones(1,N*N);
BB = ones(1,N*N-1);
BB(N:N:end) = 0;
DY2 =(-2)*diag(AA) + (1)*diag(BB,-1) + (1)*diag(BB,1);

Lap = sparse(DX2/dx^2 + DY2/dy^2);

% setting up potential
[X,Y] = meshgrid(x,y);
% harmonic potential
% U = X.^2/2 + Y.^2/2;
% strange potential
U = X.^2/2 + Y.^2/2 - sqrt(2)*abs(X-Y);

% Total Hamiltonian.
H = sparse(-(1/2)*(hbar^2/m)*Lap + diag(U(:))) ;
% Find lowest nmodes eigenvectors and eigenvalues of sparse matrix.
nmodes = 4;
[Psi,E] = eigs(H,nmodes,'SM'); % find two smallest eigenvalues <<<<<<<<<<<< use 'sr'
[E,ind] = sort(diag(E)); % convert E to vector and sort low to high.
Psi = Psi(:,ind); % rearrange corresponding eigenvectors.

% display all energies
disp('Lowest energies requested: ')
disp(E)

%%%%%%%%%%%%%%%%%%%%%%% Normalization %%%%%%%%%%%%%%%%%%%%%%%%%
for i=1:nmodes
psi_temp = reshape(Psi(:,i),N,N);
psi_result(:,:,i) = psi_temp / sqrt( trapz(y',trapz(x,abs(psi_temp).^2 ,2) , 1 ));
end

%%% NOTE: want antisymmetric \psi, so pick eigenstate #3 to plot

% plot |psi|^2 for ground state only
figure(1)
surf(X,Y,abs(psi_result(:,:,3)).^2, 'LineWidth',0.1,'edgecolor','black', 'EdgeAlpha', 0.0 , 'FaceAlpha',1)
title('|\psi|^2(x,y)')
xlabel('x')
ylabel('y')

% plot \psi for ground state only
figure(2)
surf(X,Y,psi_result(:,:,3), 'LineWidth',0.1,'edgecolor','black', 'EdgeAlpha', 0.0 , 'FaceAlpha',1)
view([0 0 90])
colorbar;
title('Antisymmetric \psi(x,y)')
xlabel('x')
ylabel('y')
```

How would one do this problem variationally? I could imagine picking sines and cosines as basis functions, but setting up the solver and minimizing the Rayleigh-Ritz quotient seem very involved. Or maybe not... I haven't tried.

Correct solution:

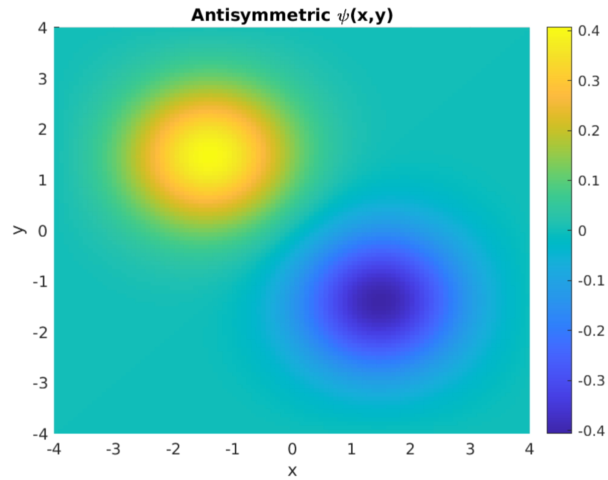


Figure 5: "Good" ground state wavefunction

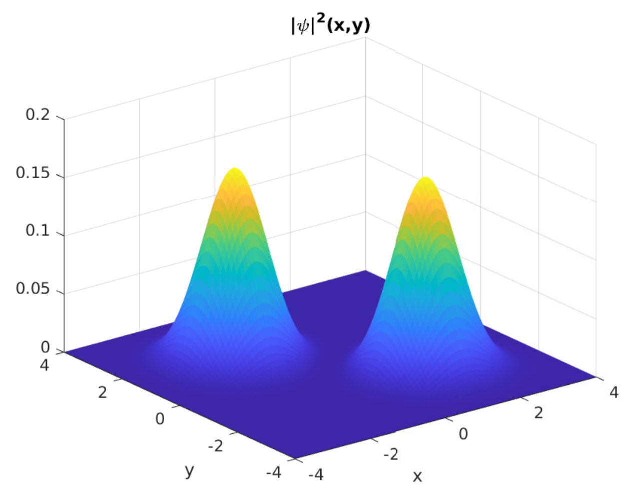


Figure 6: "Good" ground state density

(d) **(Extra credit)** Ground state energy for particle in the potential:

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

Finite difference method: I use the same approach for (c) to solve this problem. I simply modified the potential, and picked the lowest-energy state as the solution (since there's no symmetry requirement on ψ). The lowest energy is

$$\boxed{E_0 \approx 0.359}$$

MATLAB output for the 4 lowest energies:

```
Lowest energies requested:
0.3859
0.6345
1.6811
2.4703
```

The graphical solution is

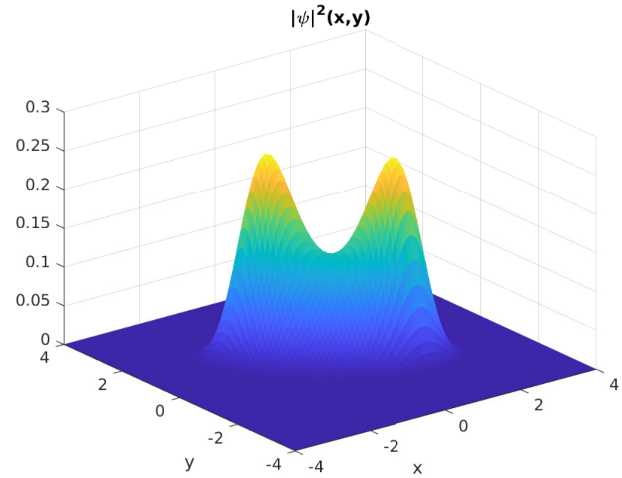


Figure 7: Ground state density function

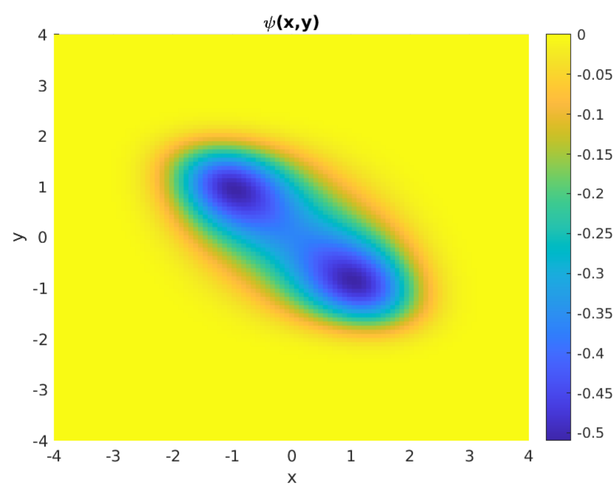


Figure 8: Ground state wavefunction