Name: **Huan Q. Bui**
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)

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

(d)

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

(e)

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

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,

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

**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

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

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 $\alpha$, 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.

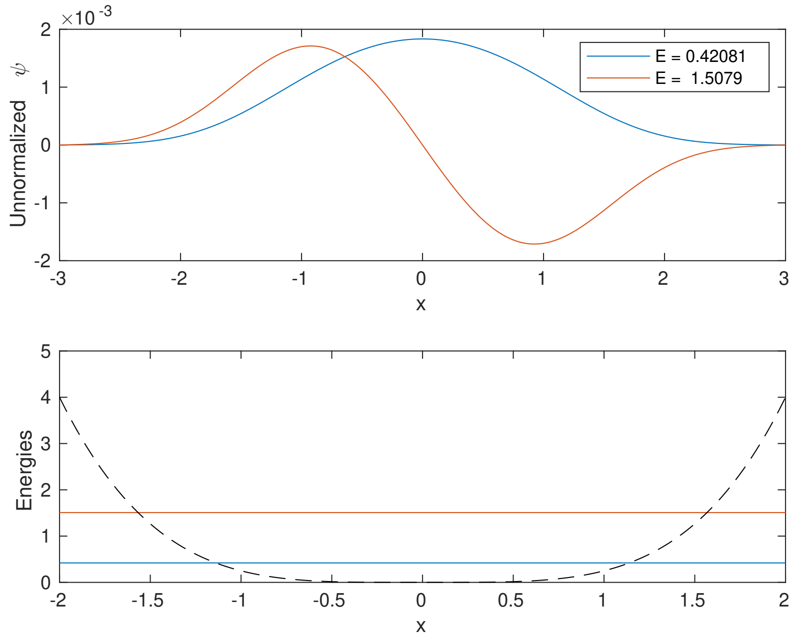
**Finite-difference method:** The Hamiltonian has the form

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

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

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

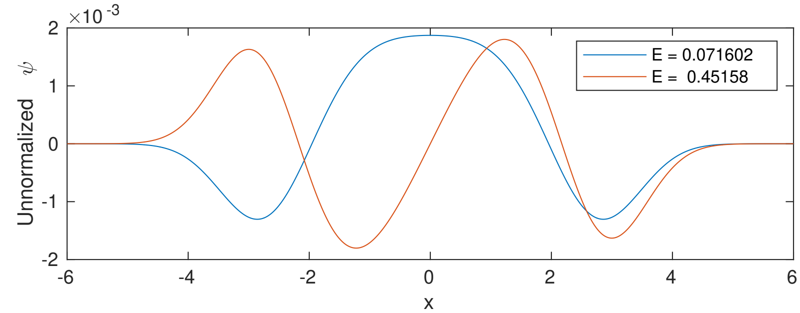
Repeating the same procedure we find

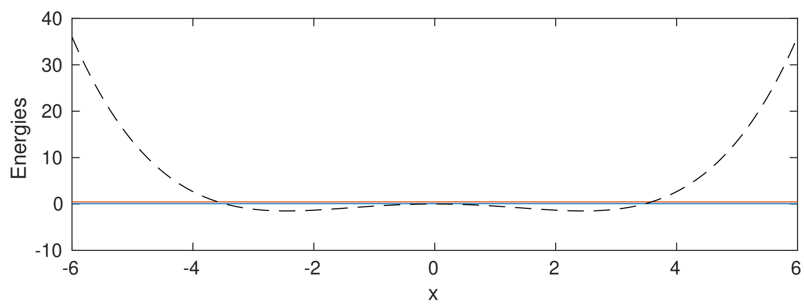
$$\boxed{E_1(\alpha) = \frac{3(5+4a^3)}{16a^2} \implies E_1 \approx \min E(\alpha) = 1.527}$$

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

(b) 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}]
```

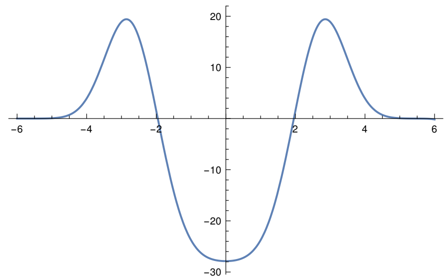



Figure 1: Ground state wavefunction

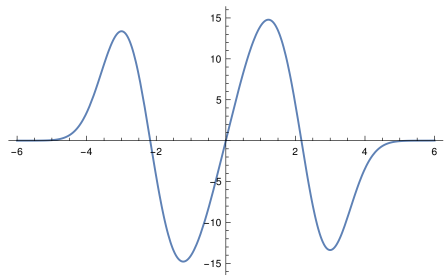



Figure 2: First excited state wavefunction

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

(c) 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 $100 \times 100$ 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 $\psi$ 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.

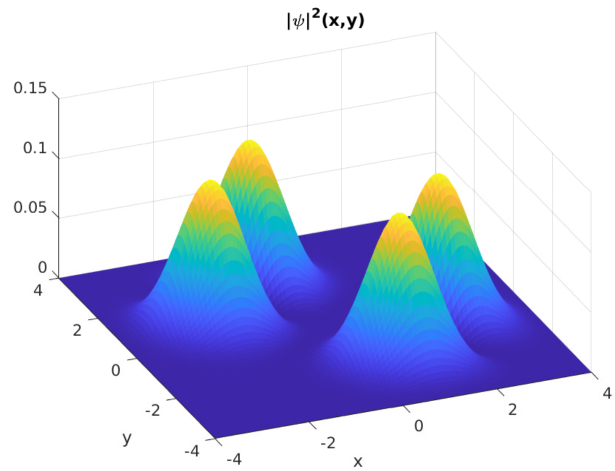



Figure 3: "Good" ground state density function

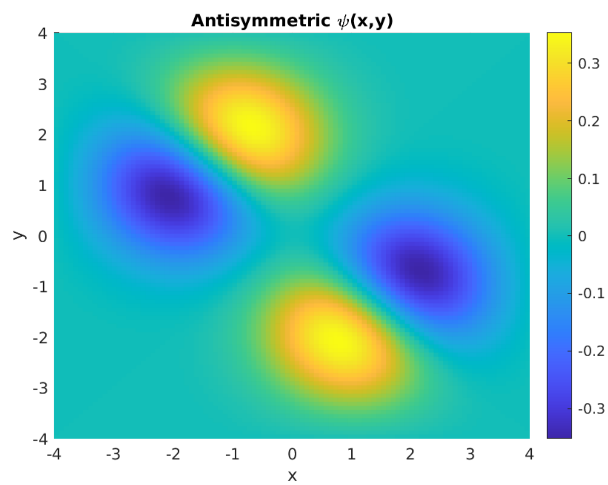



Figure 4: "Good" ground state wavefunction

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
[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.**

(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 $\psi$). 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

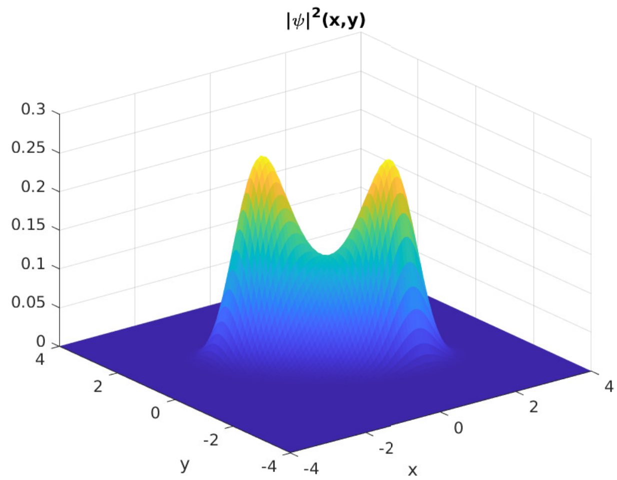



Figure 5: Ground state density function

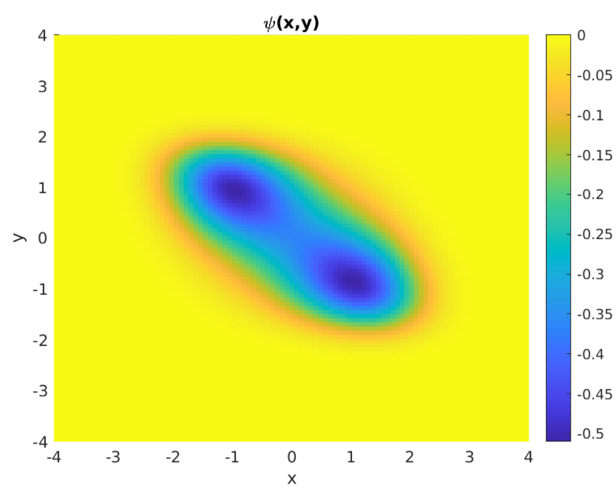



Figure 6: Ground state wavefunction