SQ16

(a) Every term in the Slater determinant is orthogonal to each other. Therefore, $\langle \psi(1,2,3) | \psi(1,2,3) \rangle = N$ where N is the number of terms in the Slater determinant. The normalization constant equals to $\frac{1}{\sqrt{N}}$.

Now, we allocate three states (a, b, c) to three particles $(1,2,3)$

The first particle has 3 choices.

The second particle has 2 choices.

The remaining particle has 1 choice.

So, there are $3 \times 2 \times 1 = 3! = 6$ terms in total.

The normalization constant is $\frac{1}{\sqrt{6}}$

$$\therefore \; \psi(1,2,3) = \frac{1}{\sqrt{6}} \begin{vmatrix} \phi_a(1) & \phi_b(1) & \phi_c(1) \\ \phi_a(2) & \phi_b(2) & \phi_c(2) \\ \phi_a(3) & \phi_b(3) & \phi_c(3) \end{vmatrix}$$

$$= \frac{1}{\sqrt{6}} \left[\phi_a(1) \begin{vmatrix} \phi_b(2) & \phi_c(2) \\ \phi_b(3) & \phi_c(3) \end{vmatrix} - \phi_b(1) \begin{vmatrix} \phi_a(2) & \phi_c(2) \\ \phi_a(3) & \phi_c(3) \end{vmatrix} \right.$$

$$\left. + \phi_c(1) \begin{vmatrix} \phi_a(2) & \phi_b(2) \\ \phi_a(3) & \phi_b(3) \end{vmatrix} \right]$$

$$= \frac{1}{\sqrt{6}} \left[\phi_a(1)\phi_b(2)\phi_c(3) - \phi_a(1)\phi_c(2)\phi_b(3) \right.$$

$$- \phi_b(1)\phi_a(2)\phi_c(3) + \phi_b(1)\phi_c(2)\phi_a(3)$$

$$\left. + \phi_c(1)\phi_a(2)\phi_b(3) - \phi_c(1)\phi_b(2)\phi_a(3) \right]$$

SQ16

(b) Interchange particle 1 and 2 :

$$\begin{aligned}\psi(2,1,3) = \frac{1}{\sqrt{6}}\Big[& \phi_a(2)\phi_b(1)\phi_c(3) - \phi_a(2)\phi_c(1)\phi_b(3) \\ & - \phi_b(2)\phi_a(1)\phi_c(3) + \phi_b(2)\phi_c(1)\phi_a(3) \\ & + \phi_c(2)\phi_a(1)\phi_b(3) - \phi_c(2)\phi_b(1)\phi_a(3)\Big] \\ = & -\psi(1,2,3)\end{aligned}$$

Actually, interchanging the coordinates of any 2 particles in a Slater determinant is equivalent to interchanging the corresponding 2 rows of the determinant, which gives an extra minus sign according to the property of a determinant.

(c) If 2 particles are in the same state, for example, the state a, the Slater determinant becomes :

$$\frac{1}{\sqrt{6}}\begin{vmatrix} \phi_a(1) & \phi_a(1) & \phi_c(1) \\ \phi_a(2) & \phi_a(2) & \phi_c(2) \\ \phi_a(3) & \phi_a(3) & \phi_c(3) \end{vmatrix},$$

which equals to 0.

The wavefunction vanishes if any 2 particles are in the same state. In other words, we cannot have 2 particles (electrons) occupying the same state.

This is exactly the "Pauli Exclusion Principle".

SQ16

(d)

$$\psi(1,2,3) = \frac{1}{\sqrt{3!}} \sum_{P} (-1)^P P \phi_a(1) \phi_b(2) \phi_c(3)$$

All possible permutations of the 3 coordinates :

even : $(1,2,3)$ $(3,1,2)$ $(2,3,1)$

odd : $(1,3,2)$ $(3,2,1)$ $(2,1,3)$

$\therefore$ $\psi(1,2,3)$

$$= \frac{1}{\sqrt{6}} \Big[\phi_a(1)\phi_b(2)\phi_c(3) + \phi_a(3)\phi_b(1)\phi_c(2) + \phi_a(2)\phi_b(3)\phi_c(1) - \phi_a(1)\phi_b(3)\phi_c(2) - \phi_a(3)\phi_b(2)\phi_c(1) - \phi_a(2)\phi_b(1)\phi_c(3) \Big]$$

which is the same as what we obtained by Slater determinant.

Any even (odd) permutation can be obtained by an even (odd) number of transpositions on $(1,2,3)$.

For example,

$(1,2,3) \to (1,3,2) \to (3,1,2)$

So, $(3,1,2)$ is even

SQ16

(e) When 2 fermions take on the same location in real space (i.e. $\vec{r}_1 = \vec{r}_2$)

$$\psi(\vec{r}_1, \vec{r}_1, \vec{r}_3) = \frac{1}{\sqrt{6}} \begin{vmatrix} \phi_a(\vec{r}_1) & \phi_b(\vec{r}_1) & \phi_c(\vec{r}_1) \\ \phi_a(\vec{r}_1) & \phi_b(\vec{r}_1) & \phi_c(\vec{r}_1) \\ \phi_a(\vec{r}_3) & \phi_b(\vec{r}_3) & \phi_c(\vec{r}_3) \end{vmatrix} = 0$$

Since $|\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)|^2 d^3r_1\, d^3r_2\, d^3r_3$ is the probability density of 3 fermions located at $\vec{r}_1$, $\vec{r}_2$ and $\vec{r}_3$ respectively, $\psi(\vec{r}_1, \vec{r}_1, \vec{r}_3) = 0$ shows that we cannot have more than one fermion located at the same location in real space.

(f)
$$\begin{aligned}\psi_S(1,2,3) &= \frac{1}{\sqrt{6}} \Big[\phi_a(1)\phi_b(2)\phi_c(3) + \phi_a(1)\phi_c(2)\phi_b(3) \\ &\quad + \phi_b(1)\phi_a(2)\phi_c(3) + \phi_b(1)\phi_c(2)\phi_a(3) \\ &\quad + \phi_c(1)\phi_a(2)\phi_b(3) + \phi_c(1)\phi_b(2)\phi_a(3) \Big] \\ &= \frac{1}{\sqrt{3!}} \sum_P (+1)^P\, P\, \phi_a(1)\phi_b(2)\phi_c(3)\end{aligned}$$

SQ17

(a)

$$\psi(x_1,x_2) = \phi_0(x_1)\,\phi_0(x_2)$$

$\phi_0(x)$: Ground state of H.O.

$$= \sqrt{\frac{m\omega_0}{\pi\hbar}}\; e^{-\frac{m\omega_0}{2\hbar}(x_1^2+x_2^2)}$$

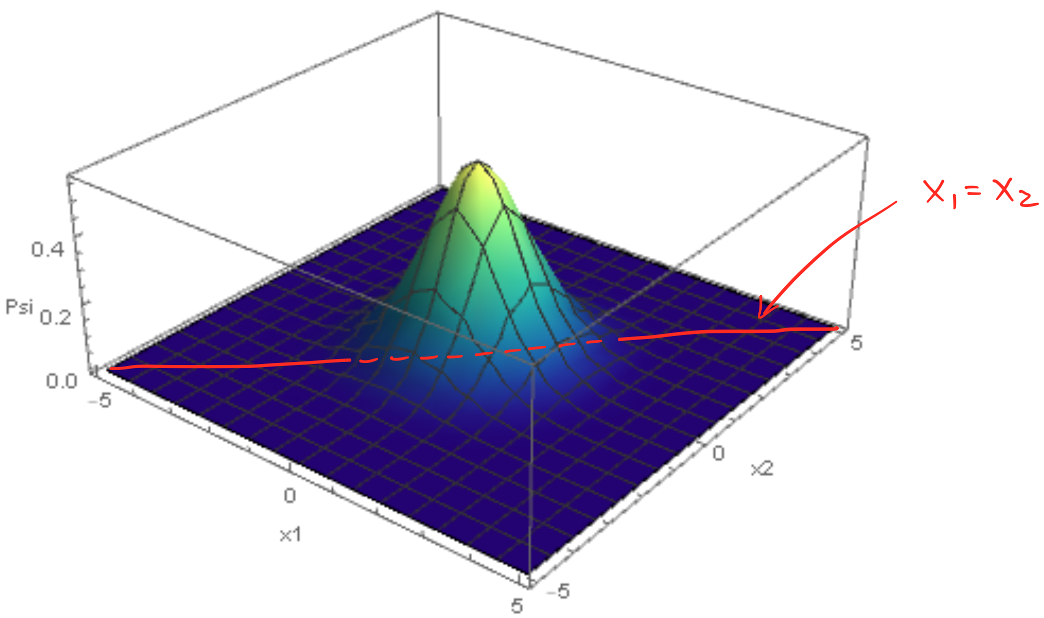
$$\psi(x_2,x_1) = \sqrt{\frac{m\omega_0}{\pi\hbar}}\; e^{-\frac{m\omega_0}{2\hbar}(x_2^2+x_1^2)}$$

$$= \psi(x_1,x_2)$$

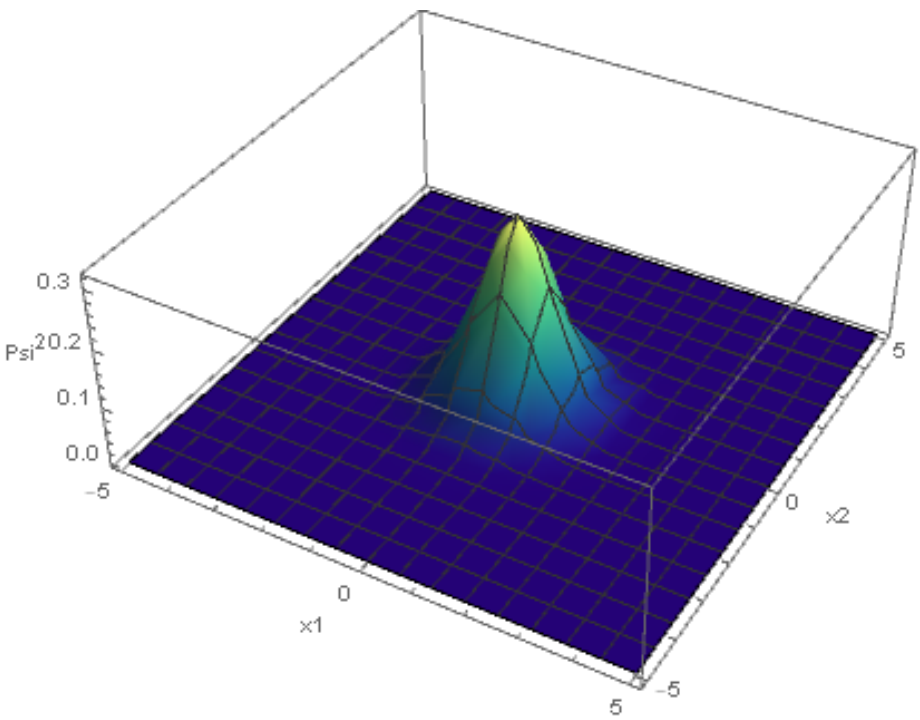
$\Rightarrow$ $\psi(x_1,x_2)$ is symmetric

(b)

$\boxed{\text{Take } m\omega_0 = \hbar \text{ in plots}}$



$\psi(x_1,x_2)$



$|\psi(x_1,x_2)|^2$

SQ17

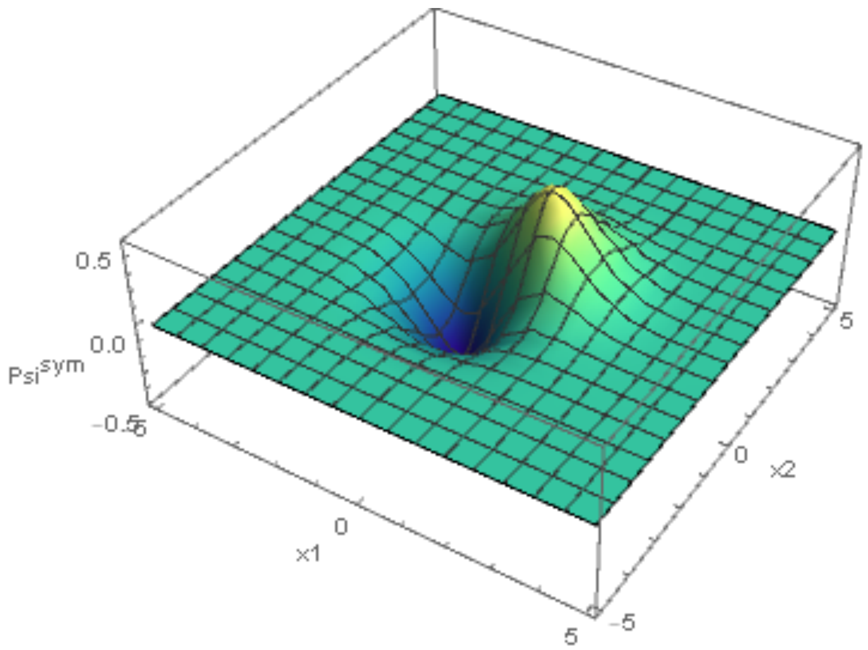
(b) A symmetric $\psi(x_1,x_2)$ means, if we draw a line $x_1=x_2$, the plot of $\psi(x_1,x_2)$ on both sides of the line is the same. (See previous page)

(c)

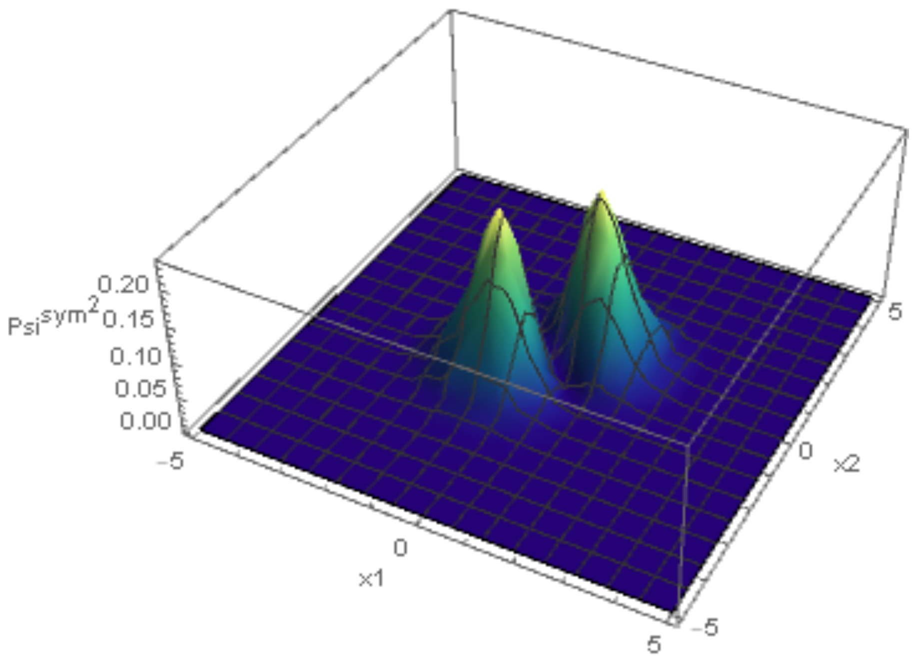
$$\psi^{(sym)}(x_1,x_2) = \frac{1}{\sqrt{2}}\left[\phi_0(x_1)\,\phi_1(x_2) + \phi_0(x_2)\,\phi_1(x_1)\right]$$

ϕ_1 : 1st excited state of H.O.

$$= \frac{1}{\sqrt{2}}\,\frac{m\omega_0}{\hbar}\sqrt{\frac{2}{\pi}}\;e^{-\frac{m\omega_0}{2\hbar}(x_2^2+x_1^2)}\;(x_2+x_1)$$



$\psi^{(sym)}(x_1,x_2)$



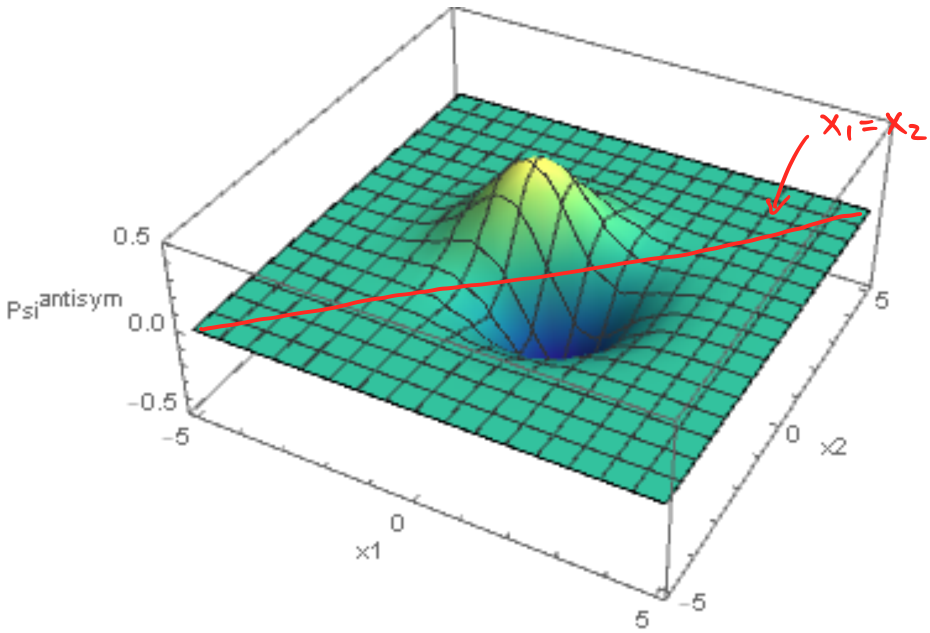
$|\psi^{(sym)}(x_1,x_2)|^2$

SQ17

(d)

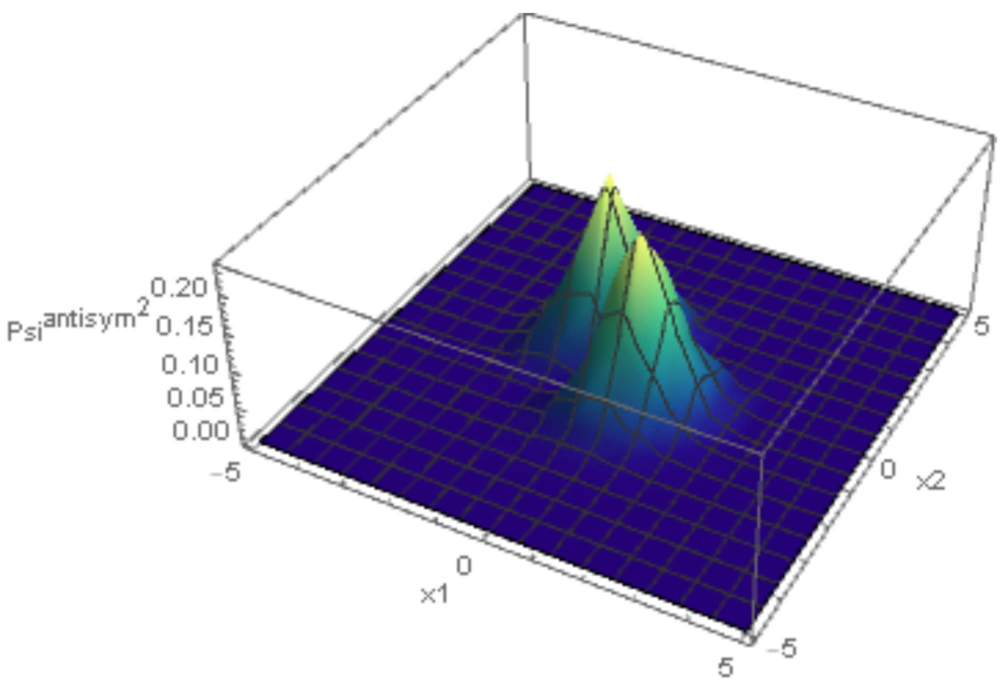
$$\psi^{(antisym)}(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\phi_0(x_1)\,\phi_1(x_2) - \phi_0(x_2)\,\phi_1(x_1)\right]$$

$$= \frac{1}{\sqrt{2}}\,\frac{m w_0}{\hbar}\sqrt{\frac{2}{\pi}}\; e^{-\frac{m w_0}{2\hbar}(x_2^2 + x_1^2)}\,(x_2 - x_1)$$



$\psi^{(antisym)}(x_1, x_2)$

An antisymmetric $\psi^{(antisym)}(x_1, x_2)$ means the plot on both sides of the line $x_1 = x_2$ are opposite to each other

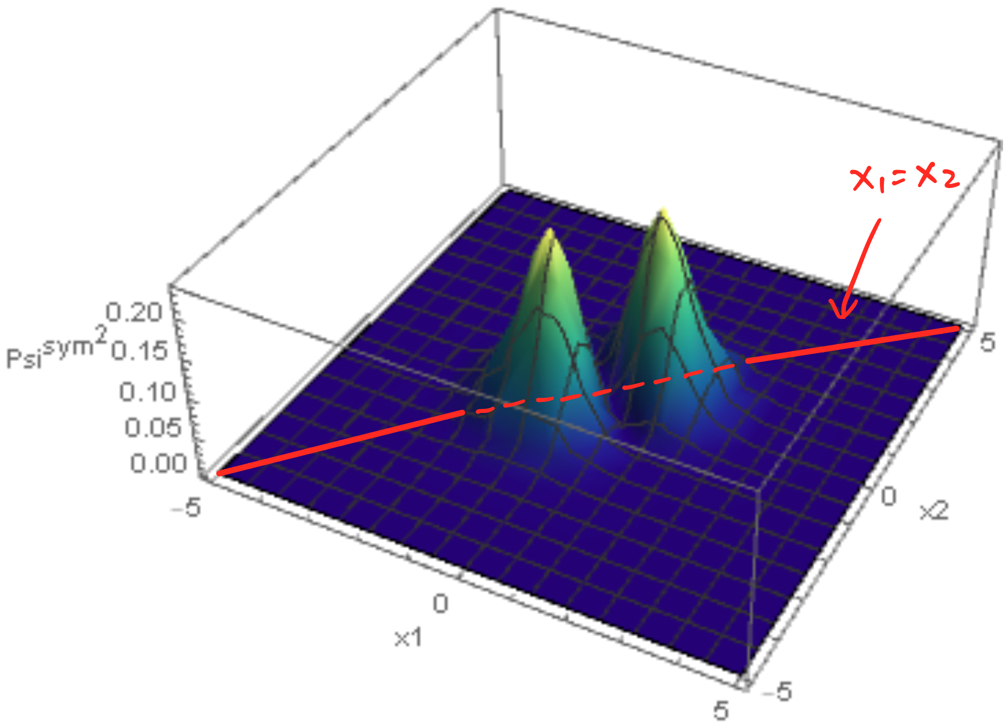


$|\psi^{(antisym)}(x_1, x_2)|^2$

SQ17

(e)

Probability density of symmetric $\psi^{(sym)}(x_1, x_2)$:



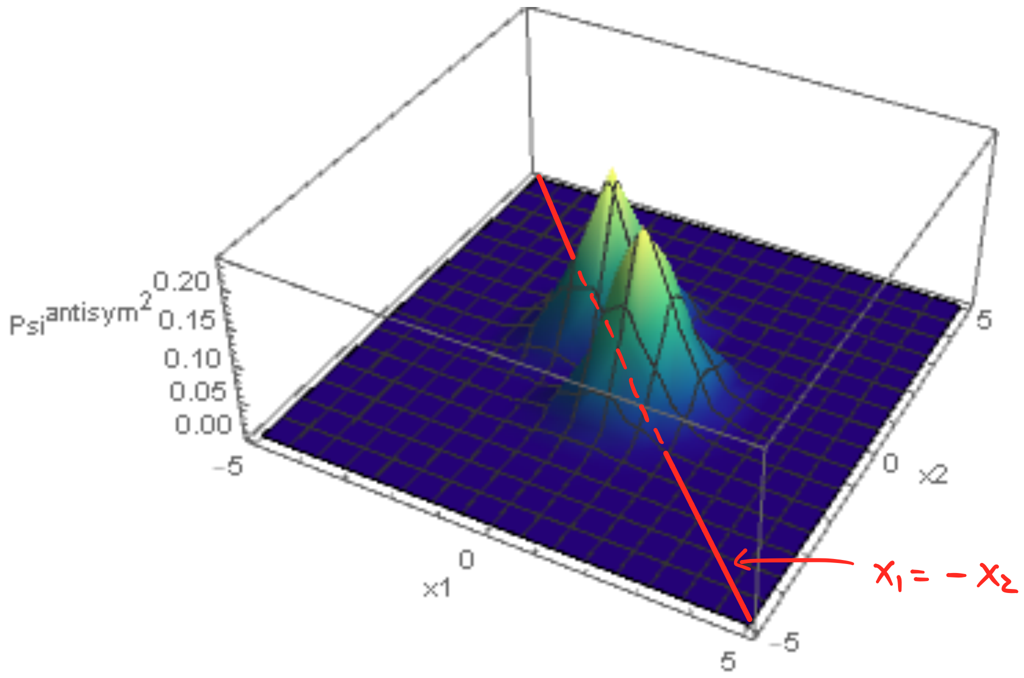
$|\psi^{(sym)}(x_1, x_2)|^2$

Two peaks of the plot lie on the line $x_1 = x_2$. One peak is at $(x_1 = \frac{1}{\sqrt{2}}, x_2 = \frac{1}{\sqrt{2}})$ while the other peak is at $(x_1 = -\frac{1}{\sqrt{2}}, x_2 = -\frac{1}{\sqrt{2}})$. This indicates that both particles tend to come together (they tend to have the same x-coordinates) for a spatially symmetric wavefunction

Sol17

(e)

Probability density of antisymmetric $\psi^{(antisym)}(x_1, x_2)$:



$|\psi^{(antisym)}(x_1, x_2)|^2$

Two peaks of the plot lie on the line $x_1 = -x_2$. One peak is at $(x_1 = \frac{1}{\sqrt{2}}, x_2 = -\frac{1}{\sqrt{2}})$ while the other peak is at $(x_1 = -\frac{1}{\sqrt{2}}, x_2 = \frac{1}{\sqrt{2}})$. This indicates that the 2 particles tend to avoid each other (they tend to have opposite x-coordinates) for a spatially antisymmetric wavefunction.