Two Particles in an Infinite Well Potential

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Abstract

Keywords:

1 Problem Setting

We consider two indistinguishable particles, each confined to a one-dimensional infinite potential well of length L. The single-particle Hilbert space is $\mathcal{H}_i \cong L^2([0, L])$. The total Hilbert space for the non-relativistic system is the tensor product of the individual spaces:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{1}$$

The configuration space is $(x_1, x_2) \in [0, L] \times [0, L]$. The potential imposes Dirichlet boundary conditions, requiring the wavefunction $\Psi(x_1, x_2)$ to vanish at the boundaries.

The system's dynamics are governed by the Hamiltonian $\hat{H}$, which we decompose into kinetic, external potential, and interaction terms:

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{int}}. \tag{2}$$

The total kinetic energy $\hat{T} = \hat{T}_1 + \hat{T}_2$ is the sum of the single-particle operators,

$$\hat{T}_1 = \frac{\hat{p}_1^2}{2m} \otimes \hat{I}, \tag{3}$$

$$\hat{T}_2 = \hat{I} \otimes \frac{\hat{p}_2^2}{2m}, \tag{4}$$

where $\hat{I}$ is the identity operator on the single-particle space.

The external potential $\hat{V}_{\text{ext}}$ is zero within the well and infinite otherwise, a constraint already enforced by the boundary conditions. The particles interact via a contact potential $\hat{V}_{\text{int}}$, which is proportional to a Dirac delta function:

$$\hat{V}_{\text{int}}(x_1, x_2) = g\,\delta(x_1 - x_2). \tag{5}$$

Here, g represents the coupling strength of the interaction.

In the position representation, the Hamiltonian operator acts on the wavefunction as

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\partial_{x_1}^2 + \partial_{x_2}^2\right) + g\,\delta(x_1 - x_2). \tag{6}$$

The configuration space is the square $[0, L] \times [0, L]$, and the interaction $\hat{V}_{\text{int}}$ is active only along the diagonal $x_1 = x_2$.

2 Symmetry and Indistinguishability

The indistinguishability of the particles implies a fundamental symmetry. We introduce the particle exchange operator $\hat{P}_{12}$, whose action on the two-particle wavefunction is defined as

$$\hat{P}_{12}\Psi(x_1, x_2) = \Psi(x_2, x_1). \tag{7}$$

This operator commutes with the Hamiltonian, $[\hat{P}_{12}, \hat{H}] = 0$, as both the kinetic term and the interaction term are symmetric under the exchange $x_1 \leftrightarrow x_2$. This commutation is a crucial property: it ensures that the exchange symmetry of a state is conserved over time. Consequently, eigenstates of $\hat{H}$ can be chosen as simultaneous eigenstates of $\hat{P}_{12}$ with eigenvalues $p_{12} = \pm 1$.

- **Bosons (Symmetric):** $p_{12} = +1$. $\Psi_S(x_1, x_2) = \Psi_S(x_2, x_1)$.
- **Fermions (Antisymmetric):** $p_{12} = -1$. $\Psi_A(x_1, x_2) = -\Psi_A(x_2, x_1)$.

The Spin-Statistics Theorem connects this symmetry to the particle's intrinsic spin. In this work, we restrict our analysis to the fermionic case, requiring the total wavefunction to be antisymmetric under particle exchange.

The state vector must therefore belong to the antisymmetric subspace $\mathcal{H}_A \subset \mathcal{H}$. For a state constructed from two distinct single-particle orbitals, $|\phi_a\rangle$ and $|\phi_b\rangle$, the normalized antisymmetric state is

$$|\Psi_A\rangle = \frac{1}{\sqrt{2}}\left(|\phi_a\rangle \otimes |\phi_b\rangle - |\phi_b\rangle \otimes |\phi_a\rangle\right). \tag{8}$$

In this notation, the first ket in each product refers to particle 1 and the second to particle 2.

Projecting eq. (8) into the position basis ($\Psi_A(x_1, x_2) = \langle x_1, x_2|\Psi_A\rangle$) yields the Slater determinant for the wavefunction:

$$\Psi_A(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\phi_a(x_1)\phi_b(x_2) - \phi_b(x_1)\phi_a(x_2)\right). \tag{9}$$

Note that if $|\phi_a\rangle = |\phi_b\rangle$, the state vanishes, in accordance with the Pauli Exclusion Principle.

3 Position Representation of Schrödinger Equation

The dynamics of the fermionic system are described by the time-dependent Schr"odinger equation. In the position representation, the equation reads:

$$i\hbar\frac{\partial}{\partial t}\Psi_A(x_1,x_2,t) = \left[-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) + g, \delta(x_1-x_2)\right]\Psi_A(x_1,x_2,t). \tag{10}$$

5. Separation of Variables and Ansatz

We look for separable solutions in space and time as our first ansatz, of the form:

$$\Psi(x_1,x_2,t) = \Psi_{n,\kappa}(x_1,x_2), \phi_t(t). \tag{11}$$

To construct an antisymmetric spatial function for fermions, we use two single-particle eigenfunctions, $\phi_n(x)$ and $\phi_\kappa(x)$, and combine them as follows:

$$\Psi_F(x_1,x_2,t) = \frac{1}{\sqrt{2}}\left[\phi_n(x_1)\phi_\kappa(x_2) - \phi_n(x_2)\phi_\kappa(x_1)\right]\phi_t(t), \tag{12}$$

which correctly satisfies the antisymmetry condition required for fermionic states. where the single-particle functions (our second ansatz) are given by:

$$\phi_n(x_i) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x_i}{L}\right), \tag{13}$$

and the temporal factor corresponds to the usual energy eigenstate exponential, a result of the separable form of the time-dependent Schrödinger equation:

$$\phi_t(t) = e^{-iEt/\hbar}. \tag{14}$$

Substituting both expressions into the fermionic ansatz, we obtain the complete wavefunction:

$$\Psi_F(x_1,x_2,t) = \sqrt{\frac{1}{2}}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x_1}{L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\kappa\pi x_2}{L}\right) - \sqrt{\frac{2}{L}}\sin\left(\frac{\kappa\pi x_1}{L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x_2}{L}\right)\right]e^{-iEt/\hbar}. \tag{15}$$

Simplifying the prefactors, the final normalized antisymmetric fermionic wavefunction becomes:

$$\Psi_F(x_1,x_2,t) = \frac{1}{\sqrt{L^2}}\left[\sin\left(\frac{n\pi x_1}{L}\right)\sin\left(\frac{\kappa\pi x_2}{L}\right) - \sin\left(\frac{\kappa\pi x_1}{L}\right)\sin\left(\frac{n\pi x_2}{L}\right)\right]e^{-iEt/\hbar}, \tag{16}$$

4. Expectation Value of the Interaction for Fermions

The expectation value of the interaction potential $V = g\,\delta(x_1 - x_2)$ in a fermionic state is:

$$\langle\psi_F|V|\psi_F\rangle = g\int_0^L\int_0^L \psi_F^*(x_1,x_2)\,\psi_F(x_1,x_2)\,\delta(x_1-x_2)\,dx_1\,dx_2. \tag{17}$$

Because $\psi_F(x,x) = 0$ for all x in $[0, L]$, the integrand vanishes on the support of the delta distribution and therefore:

$$\langle\psi_F|V|\psi_F\rangle = 0. \tag{18}$$

5. Determination of the Energy

Substituting the ansatz into the Schrödinger equation and separating space and time yields:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi_{n,\kappa}}{\partial x_1^2} + \frac{\partial^2\Psi_{n,\kappa}}{\partial x_2^2}\right) = E\,\Psi_{n,\kappa}, \tag{19}$$

$$i\hbar\frac{1}{\phi_t}\frac{d\phi_t}{dt} = E. \tag{20}$$

Thus the spatial energy eigenvalue reads:

$$E = -\frac{\hbar^2}{2m}\frac{\left(\partial_{x_1}^2\Psi_{n,\kappa} + \partial_{x_2}^2\Psi_{n,\kappa}\right)}{\Psi_{n,\kappa}}. \tag{21}$$

Using that for the single-particle eigenfunctions $\partial_{x_i}^2\phi_n(x_i) = -n^2\omega^2\phi_n(x_i)$ with $\omega = \pi/L$, one obtains:

$$\partial_{x_1}^2\Psi_{n,\kappa} + \partial_{x_2}^2\Psi_{n,\kappa} = -\omega^2(n^2+\kappa^2)\Psi_{n,\kappa}. \tag{22}$$

Hence the energy associated with the two-particle antisymmetric state is:

$$E = \frac{\hbar^2\omega^2}{2m}(n^2+\kappa^2) = \frac{\pi^2\hbar^2}{2mL^2}(n^2+\kappa^2). \tag{23}$$

6. Final Form of the Wavefunction

The complete fermionic wavefunction for the considered state is therefore:

$$\Psi_F(x_1,x_2,t) = \frac{1}{\sqrt{2}}\left[\sin\left(\frac{n\pi x_1}{L}\right)\sin\left(\frac{\kappa\pi x_2}{L}\right) - \sin\left(\frac{\kappa\pi x_1}{L}\right)\sin\left(\frac{n\pi x_2}{L}\right)\right]e^{-iEt/\hbar}, \tag{24}$$

with E given above.

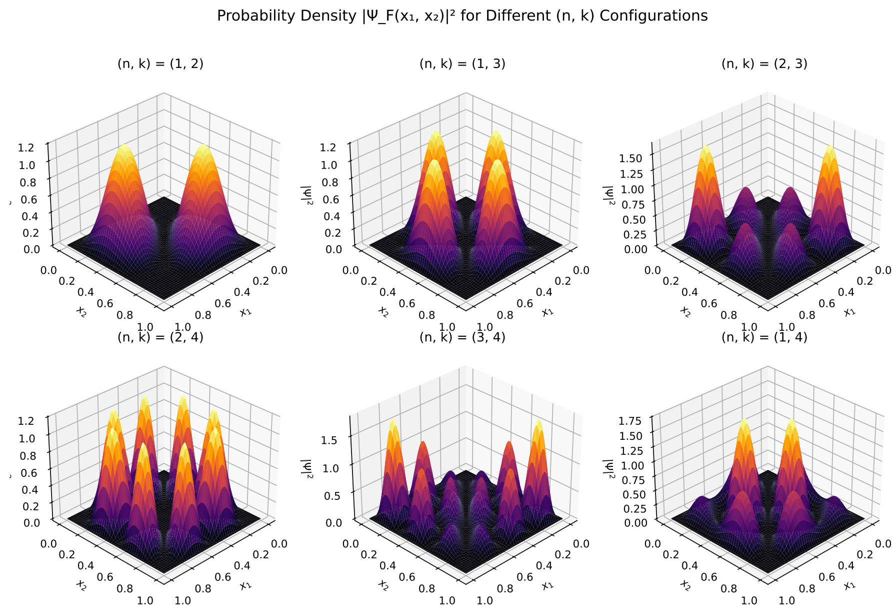

Fig. 1 Probability density $|\Psi_F(x_1, x_2)|^2$ for six antisymmetric two-fermion configurations $(n, \kappa) = (1,2), (1,3), (2,3), (2,4), (3,4), (1,4)$. The antisymmetric nature of the wavefunction enforces $\Psi_F(x_1 = x_2) = 0$, reflecting the Pauli exclusion principle.

4 Remarks and Validity

The derivation above is valid for the antisymmetric spatial sector (fermions) and for the idealized contact interaction represented by the delta potential. For bosonic states, the delta interaction generally yields nontrivial corrections to energy eigenvalues and must be treated using either regularization methods or matching conditions across the line $x_1 = x_2$. The present fermionic ansatz trivially nullifies the delta contribution because of the vanishing of the wavefunction at coincidence points.