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

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\partial_1^2 + \partial_2^2\right) + g\,\delta(x_1 - x_2). \tag{6}$$

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 the Schrödinger Equation

The dynamics are governed by the time-dependent Schrödinger equation (TDSE). In the position representation, using the Hamiltonian from eq. (6), this reads:

$$i\hbar\partial_t\Psi(x_1, x_2, t) = \left(-\frac{\hbar^2}{2m}(\partial_1^2 + \partial_2^2) + g\delta(x_1 - x_2)\right)\Psi(x_1, x_2, t). \tag{10}$$

A central consequence of the fermionic symmetry, discussed in section 2, is the antisymmetry of the wavefunction: $\Psi(x_1, x_2, t) = -\Psi(x_2, x_1, t)$. This requirement has a profound effect on the interaction term. If we evaluate the wavefunction along the diagonal $x_1 = x_2 = x$, the antisymmetry implies

$$\Psi(x, x, t) = -\Psi(x, x, t) \quad \Longrightarrow \quad \Psi(x, x, t) = 0. \tag{11}$$

The wavefunction must be identically zero for any configuration where the two particles are at the same position.

Because the delta-function potential $\hat{V}_{\text{int}} = g\delta(x_1 - x_2)$ has support only on this diagonal (where the wavefunction vanishes), the interaction term has no effect on the system. We can confirm this by examining the expected value of the interaction potential:

$$\begin{aligned}
\langle\hat{V}_{\text{int}}\rangle &= \langle\Psi|g\delta(x_1 - x_2)|\Psi\rangle \\
&= g\int_0^L\int_0^L \Psi^*(x_1, x_2)\Psi(x_1, x_2)\delta(x_1 - x_2)\,\mathrm{d}x_2\mathrm{d}x_1 \\
&= g\int_0^L \Psi^*(x_1, x_1)\Psi(x_1, x_1)\,\mathrm{d}x_1 \\
&= g\int_0^L |0|^2\,\mathrm{d}x_1 = 0.
\end{aligned} \tag{12}$$

Therefore, for fermions, the problem simplifies remarkably. The system behaves as two non-interacting identical particles in an infinite well, and the governing equation reduces to

$$i\hbar\partial_t\Psi(x_1, x_2, t) = -\frac{\hbar^2}{2m}\left(\partial_1^2 + \partial_2^2\right)\Psi(x_1, x_2, t). \tag{13}$$

We seek stationary-state solutions by applying the separation of variables, positing an ansatz of the form

$$\Psi(x_1, x_2, t) = \psi(x_1, x_2)\varphi(t). \tag{14}$$

Substituting this into eq. (13) and dividing by $\Psi(x_1, x_2, t)$ separates the spatial and temporal components:

$$\frac{1}{\psi(x_1,x_2)}\left[-\frac{\hbar^2}{2m}(\partial_1^2+\partial_2^2)\right]\psi(x_1,x_2) = i\hbar\frac{1}{\varphi(t)}\mathrm{D}_t\varphi. \tag{15}$$

The left side depends only on position and the right side only on time, so both must equal a separation constant, which we identify as the total energy E. This yields two independent equations: the Time-Independent Schrödinger Equation (TISE)

$$\left[-\frac{\hbar^2}{2m}(\partial_1^2+\partial_2^2)\right]\psi(x_1,x_2) = E\psi(x_1,x_2), \tag{16}$$

and the temporal equation

$$i\hbar\mathrm{D}_t\varphi = E\phi(t). \tag{17}$$

3.1 Time Component

The solution to the temporal equation, eq. (17), is straightforward,

$$\varphi(t) = e^{-iEt/\hbar}, \tag{18}$$

where we have set the initial phase $\phi(0) = 1$. The full time-dependent solution for a stationary state is thus $\Psi(x_1, x_2, t) = \psi(x_1, x_2)e^{-iEt/\hbar}$. The time evolution manifests only as a global phase, which is unobservable.

3.2 Spatial Component and Energy

We now solve the spatial TISE, eq. (16). Since the Hamiltonian is a sum of non-interacting single-particle Hamiltonians ($\hat{H} = \hat{H}_1 + \hat{H}_2$), we can construct the solution from the single-particle energy eigenfunctions.

The normalized stationary states for a single particle in the well are

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots \tag{19}$$

These are eigenfunctions of the single-particle Hamiltonian, $\hat{H}_i\phi_n(x_i) = E_n\phi_n(x_i)$, with corresponding energy eigenvalues

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{20}$$

As required for fermions, we construct the two-particle spatial wavefunction as the normalized Slater determinant

$$\psi(n_1, n_2; x_1, x_2) = \frac{1}{\sqrt{2}}\left[\phi_{n_1}(x_1)\phi_{n_2}(x_2) - \phi_{n_1}(x_2)\phi_{n_2}(x_1)\right] \tag{21}$$

which is valid for $n_1 \neq n_2$, in accordance with the Pauli Exclusion Principle.

We verify this is an eigenfunction of the total spatial Hamiltonian $\hat{H} = \hat{H}_1 + \hat{H}_2$:

$$\begin{aligned}\hat{H}\psi &= (\hat{H}_1 + \hat{H}_2)\frac{1}{\sqrt{2}}\left[\phi_{n_1}(x_1)\phi_{n_2}(x_2) - \phi_{n_1}(x_2)\phi_{n_2}(x_1)\right] \\ &= (E_{n_1} + E_{n_2})\psi_{n_1,n_2}. \end{aligned} \tag{22}$$

By comparing this with the TISE, $\hat{H}\psi = E\psi$, we identify the total energy of the system as the sum of the single-particle energies:

$$E_{n_1,n_2} = E_{n_1} + E_{n_2} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2 + n_2^2). \tag{23}$$

The prefactor $1/\sqrt{2}$ in eq. (21) ensures the state is normalized ($\langle\psi|\psi\rangle = 1$) due to the orthonormality of the single-particle orbitals ϕ_n.

3.3 Visualization and Discussion

To conclude the analysis in the position representation, we visualize the probability density $|\psi(x_1, x_2)|^2$ for several low-energy stationary states.

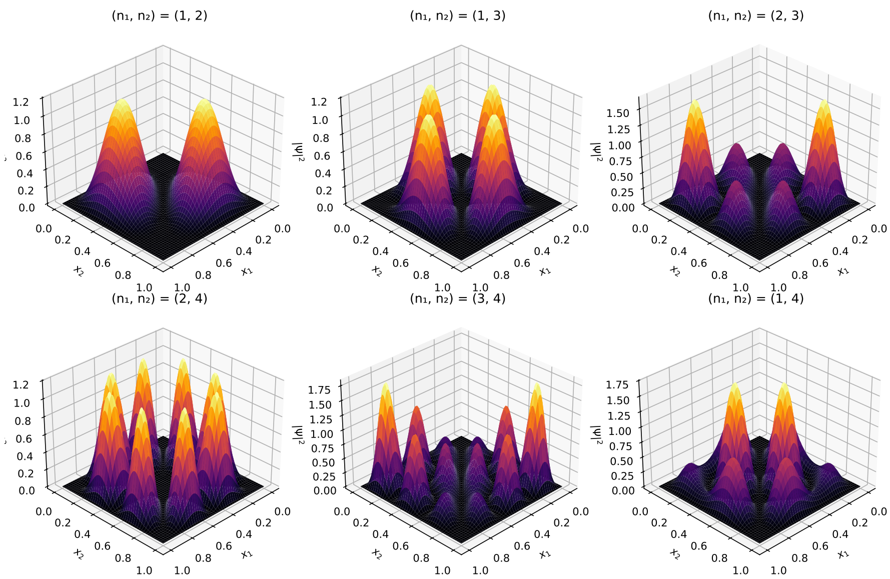

Fig. 1 Probability density $|\psi(x_1, x_2)|^2$ for six antisymmetric two-fermion configurations $\{n_1, n_2\} = \{1,2\}, \{1,3\}, \{2,3\}, \{2,4\}, \{3,4\}, \{1,4\}$.

Figure 1 illustrates the spatial characteristics of the fermionic states. Although the phase information is lost when taking the modulus squared, a "nodal line" is clearly visible along the diagonal $x_1 = x_2$, where the probability density is identically zero.

As these are stationary states, the time evolution $\Psi(x_1, x_2, t) = \psi(x_1, x_2)e^{-iEt/\hbar}$ introduces only a global phase. The probability density is therefore static: $|\Psi(x_1, x_2, t)|^2 = |\psi(x_1, x_2)|^2$.

It is crucial to contrast this result with the bosonic case. The derivation above, which led to the vanishing of the interaction, is valid only for the antisymmetric spatial sector (fermions). For bosons, the spatial wavefunction $\psi_S(x_1, x_2)$ is symmetric, so $\psi_S(x, x) \neq 0$. The delta interaction would therefore be non-trivial, yielding corrections to the energy eigenvalues.

This fermionic solution trivially nullifies the delta contribution only because we have assumed a spatially antisymmetric wavefunction. This implies the fermions are either spinless (a theoretical construct) or are in a spin-symmetric state (a triplet state), which forces the spatial part to be antisymmetric.

If, however, the two fermions (e.g., electrons) were in a spin-antisymmetric (singlet) state, the total wavefunction $|\Psi\rangle_{\text{total}} = |\psi\rangle_{\text{spatial}} \otimes |\chi\rangle_{\text{spin}}$ would require a spatially symmetric wavefunction $\psi_S(x_1, x_2)$ to maintain total antisymmetry. In that scenario, $\psi_S(x, x) \neq 0$, the delta-function interaction would apply, and the problem would become non-trivial.

4 Momentum Representation of the Schrödinger Equation

It is well-known that transforming problems with hard-wall boundaries to the momentum representation is inherently challenging. The difficulty arises not from the potential, but from the kinetic operator.

We seek the TISE by applying the 2D Fourier transform, defined over the finite domain $x_i \in [0, L]$:

$$\tilde{\psi}(p_1, p_2) = \frac{1}{2\pi\hbar} \int_0^L \int_0^L \psi(x_1, x_2) e^{-i(p_1 x_1 + p_2 x_2)/\hbar} \, \mathrm{d}x_1 \mathrm{d}x_2. \tag{24}$$

As in the position-space analysis (eq. (12)), the fermionic antisymmetry ensures $\psi(x, x) = 0$. Consequently, the interaction term $\hat{V}_{\text{int}} = g\delta(x_1 - x_2)$ has a null contribution, and the TISE in momentum space simplifies to $\mathcal{F}[\hat{T}\psi] = E\tilde{\psi}$.

The primary challenge is the kinetic operator. The Fourier transform of a second derivative over a finite domain, $\mathcal{F}[\partial_x^2 \psi]$, does not simply map to $-(p^2/\hbar^2)\tilde{\psi}(p)$. Instead, integration by parts introduces boundary terms. For simplicity, consider the 1D kinetic operator $\hat{T} = -\frac{\hbar^2}{2m}\partial_x^2$. Its Fourier transform is

$$\mathcal{F}[\hat{T}\psi](p) = \frac{p^2}{2m}\tilde{\psi}(p) - \frac{\hbar^2}{2m}\left(e^{-ipL/\hbar}\psi'(L) - \psi'(0)\right), \tag{25}$$

where $\psi'(x) \equiv \partial_x \psi(x)$ and we have used the Dirichlet conditions $\psi(0) = \psi(L) = 0$.

Generalizing to our 2D system, the TISE in momentum space becomes a complex integral equation. The transform of the kinetic term $\mathcal{F}[(\hat{T}_1 + \hat{T}_2)\psi]$ introduces terms dependent on the (unknown) derivatives of the wavefunction at all four boundaries

$(x_1 = 0, x_1 = L, x_2 = 0, x_2 = L)$.

$$\begin{split}\mathcal{F}[(\hat{T}_1 + \hat{T}_2)\psi] = \frac{1}{2m}(p_1^2 + p_2^2)\tilde{\psi}(p_1, p_2) - \frac{\hbar^2}{2m}\left(e^{-ip_1L/\hbar}\partial_1\psi(L, x_2) - \partial_2\psi(0, x_2)\right) - \\ - \frac{\hbar^2}{2m}\left(e^{-ip_2L/\hbar}\partial_2\psi(x_1, L) - \partial_2\psi(x_1, 0)\right)\end{split} \tag{26}$$

This TISE becomes an integral equation whose kernel depends on these unknown boundary values (e.g., $\partial_1\psi(L, x_2)$). Solving this is notoriously difficult and requires advanced techniques, such as Green's functions or treating the infinite well as the limit of a finite potential. Given these complexities, which obscure the simple physics derived in the position representation, we will not pursue the momentum-space solution further.