Fermion Operators

Contents

1 Anticommutation

Consider the following eigenstates of a hypothetical quantum system.[1]

$\lvert 00\rangle = (1\ 0\ 0\ 0)^\dagger$	no fermions
$\lvert 10\rangle = (0\ 1\ 0\ 0)^\dagger$	one fermion in state 1
$\lvert 01\rangle = (0\ 0\ 1\ 0)^\dagger$	one fermion in state 2
$\lvert 11\rangle = (0\ 0\ 0\ 1)^\dagger$	two fermions, one in state 1, one in state 2

Creation and annihilation operators are formed from outer products of state vectors. Sign changes make the operators antisymmetric.

$\hat{b}_1^\dagger = \lvert 10\rangle\langle 00\rvert - \lvert 11\rangle\langle 01\rvert$	Create one fermion in state 1
$\hat{b}_1 = \lvert 00\rangle\langle 10\rvert - \lvert 01\rangle\langle 11\rvert$	Annihilate one fermion in state 1
$\hat{b}_2^\dagger = \lvert 01\rangle\langle 00\rvert + \lvert 11\rangle\langle 10\rvert$	Create one fermion in state 2
$\hat{b}_2 = \lvert 00\rangle\langle 01\rvert + \lvert 10\rangle\langle 11\rvert$	Annihilate one fermion in state 2

The operators in matrix form.

$$\hat{b}_1^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix} \quad \hat{b}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \hat{b}_2^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \hat{b}_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Verify anticommutation relations of the operators.

$$\hat{b}_j\hat{b}_k + \hat{b}_k\hat{b}_j = 0$$

$$\hat{b}_j^\dagger\hat{b}_k^\dagger + \hat{b}_k^\dagger\hat{b}_j^\dagger = 0$$

$$\hat{b}_j\hat{b}_k^\dagger + \hat{b}_k^\dagger\hat{b}_j = \delta_{jk}$$

[1] Adapted from problem 16.1.1 of "Quantum Mechanics for Scientists and Engineers."
`https://ee.stanford.edu/~dabm/QMbook.html`

2 Wavefunction operator

Consider the following eigenstates of a hypothetical quantum system.[2]

$$
\begin{aligned}
&|00\rangle = (1\ 0\ 0\ 0)^\dagger && \text{no fermions} \\
&|10\rangle = (0\ 1\ 0\ 0)^\dagger && \text{one fermion in state } \phi_1 \\
&|01\rangle = (0\ 0\ 1\ 0)^\dagger && \text{one fermion in state } \phi_2 \\
&|11\rangle = (0\ 0\ 0\ 1)^\dagger && \text{two fermions, one in state } \phi_1\text{, one in state } \phi_2
\end{aligned}
$$

Let fermion states ϕ_n be modeled by a one dimensional box of length L.

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Creation and annihilation operators are formed from outer products of state vectors. Sign changes make the operators antisymmetric.

$$
\begin{aligned}
&\hat{b}_1^\dagger = |10\rangle\langle 00| - |11\rangle\langle 01| && \text{Create one fermion in state } \phi_1 \\
&\hat{b}_1 = |00\rangle\langle 10| - |01\rangle\langle 11| && \text{Annihilate one fermion in state } \phi_1 \\
&\hat{b}_2^\dagger = |01\rangle\langle 00| + |11\rangle\langle 10| && \text{Create one fermion in state } \phi_2 \\
&\hat{b}_2 = |00\rangle\langle 01| + |10\rangle\langle 11| && \text{Annihilate one fermion in state } \phi_2
\end{aligned}
$$

Given the wavefunction operator

$$\hat{\psi} = \frac{1}{\sqrt{2}} \sum_{n,m} \phi_n(x)\phi_m(y)\hat{b}_n\hat{b}_m$$

show that

$$\hat{\psi}|11\rangle = \frac{1}{\sqrt{2}}\big(\phi_1(x)\phi_2(y) - \phi_1(y)\phi_2(x)\big)|00\rangle$$

[2]Adapted from problem 16.2.1 of "Quantum Mechanics for Scientists and Engineers." `https://ee.stanford.edu/~dabm/QMbook.html`

3 Position operator

Consider the following eigenstates of a hypothetical quantum system.

$$
\begin{aligned}
|00\rangle &= (1\ 0\ 0\ 0)^\dagger && \text{no fermions} \\
|10\rangle &= (0\ 1\ 0\ 0)^\dagger && \text{one fermion in state } \phi_1 \\
|01\rangle &= (0\ 0\ 1\ 0)^\dagger && \text{one fermion in state } \phi_2 \\
|11\rangle &= (0\ 0\ 0\ 1)^\dagger && \text{two fermions, one in state } \phi_1\text{, one in state } \phi_2
\end{aligned}
$$

Let fermion states ϕ_n be modeled by a one dimensional box of length L.

$$
\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)
$$

Creation and annihilation operators are formed from outer products of state vectors. Sign changes make the operators antisymmetric.

$$
\begin{aligned}
\hat{b}_1^\dagger &= |10\rangle\langle 00| - |11\rangle\langle 01| && \text{Create one fermion in state } \phi_1 \\
\hat{b}_1 &= |00\rangle\langle 10| - |01\rangle\langle 11| && \text{Annihilate one fermion in state } \phi_1 \\
\hat{b}_2^\dagger &= |01\rangle\langle 00| + |11\rangle\langle 10| && \text{Create one fermion in state } \phi_2 \\
\hat{b}_2 &= |00\rangle\langle 01| + |10\rangle\langle 11| && \text{Annihilate one fermion in state } \phi_2
\end{aligned}
$$

Let $\hat{r}$ be the position operator

$$
\hat{r} = \sum_{n,m} r_{nm} \hat{b}_n^\dagger \hat{b}_m
$$

where

$$
r_{nm} = \int_0^L \phi_n^*(x) x \phi_m(x)\, dx
$$

Note that for a one dimensional box

$$
r_{nn} = \langle x \rangle = \tfrac{1}{2} L
$$

Verify that

$$
\begin{aligned}
\langle 10|\hat{r}|10\rangle &= r_{11} \\
\langle 10|\hat{r}|01\rangle &= r_{12} \\
\langle 01|\hat{r}|10\rangle &= r_{21} \\
\langle 01|\hat{r}|01\rangle &= r_{22}
\end{aligned}
$$

4 Exchange energy

Let $\psi(x,y)$ be the antisymmetrized wave function for two electrons in a box of length L.

$$\psi(x,y) = \frac{1}{\sqrt{2}}\big(\phi_1(x)\phi_2(y) - \phi_1(y)\phi_2(x)\big)$$

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

For $L = 10^{-9}$ meter the expected potential energy is

$$V = \frac{e^2}{4\pi\epsilon_0}\int_0^L\int_0^L \frac{\psi^*(x,y)\psi(x,y)}{|x-y|}\,dx\,dy = 4.67\,\mathrm{eV}$$

Next calculate the potential energy for a wave function that is not antisymmetrized.

$$V_0 = \frac{e^2}{4\pi\epsilon_0}\int_0^L\int_0^L \frac{\phi_1^*(x)\phi_2^*(y)\phi_1(x)\phi_2(y)}{|x-y|}\,dx\,dy = 12.80\,\mathrm{eV}$$

The difference is the exchange energy.

$$V_{ex} = V - V_0 = -8.13\,\mathrm{eV}$$

Note that the formula for V_0 has a singularity at $x = y$. The computed value shown above is the result of an arbitrary cutoff in numerical integration. The actual value of V_0 goes to infinity.

Note also that there is a singularity at $x = y$ in the formula for V. However, due to antisymmetry we have $\psi(x,x) = 0$ and hence the integral converges.

We are left to ponder the reality of exchange energy since it cannot be computed.

5 Energy matrix

Consider a system with the following eigenstates.

$$
\begin{array}{ll}
|0\rangle = (1\ 0\ 0\ 0)^\dagger & \text{no electrons} \\
|1\rangle = (0\ 1\ 0\ 0)^\dagger & \text{one electron in state } \phi_1 \\
|2\rangle = (0\ 0\ 1\ 0)^\dagger & \text{one electron in state } \phi_2 \\
|3\rangle = (0\ 0\ 0\ 1)^\dagger & \text{two electrons, one in state } \phi_1\text{, one in state } \phi_2
\end{array}
$$

Let electron states ϕ_n be modeled by a one dimensional box of length L.

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Let $|\xi\rangle$ be an arbitrary normalized state vector.

$$|\xi\rangle = c_0|0\rangle + c_1|1\rangle + c_2|2\rangle + c_3|3\rangle, \qquad \langle\xi|\xi\rangle = 1$$

Let us determine an energy matrix $\hat{E}$ such that the expected energy $\langle E\rangle$ in state $|\xi\rangle$ is

$$\langle E\rangle = \langle\xi|\hat{E}|\xi\rangle$$

Energy matrix $\hat{E}$ is the sum of kinetic and potential energy matrices.

$$\hat{E} = \hat{K} + \hat{V}$$

Kinetic energy matrix $\hat{K}$ can be computed from energy eigenvalues of the box model.

$$\hat{K} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & E_1 & 0 & 0 \\ 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & E_1 + E_2 \end{pmatrix}, \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Potential energy matrix $\hat{V}$ has one entry due to Coulomb interaction in the two electron state.

$$\hat{V} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & V \end{pmatrix}$$

Let $\psi(x,y)$ be the antisymmetrized wavefunction of the two electrons.

$$\psi(x,y) = \frac{1}{\sqrt{2}}\big(\phi_1(x)\phi_2(y) - \phi_1(y)\phi_2(x)\big)$$

Then

$$V = \frac{e^2}{4\pi\epsilon_0} \int_0^L \int_0^L \psi^*(x,y) \left(\frac{1}{|x-y|}\right) \psi(x,y)\, dx\, dy$$

Let us now choose $L = 10^{-9}$ meters and compute numerical values. For $\hat{K}$ we have

$$\hat{K} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.38\,\mathrm{eV} & 0 & 0 \\ 0 & 0 & 1.50\,\mathrm{eV} & 0 \\ 0 & 0 & 0 & 1.88\,\mathrm{eV} \end{pmatrix}$$

Computing V by numerical integration we have

$$\hat{V} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.67\,\mathrm{eV} \end{pmatrix}$$

Hence

$$\hat{E} = \hat{K} + \hat{V} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.38\,\mathrm{eV} & 0 & 0 \\ 0 & 0 & 1.50\,\mathrm{eV} & 0 \\ 0 & 0 & 0 & 6.55\,\mathrm{eV} \end{pmatrix}$$

6 Superposition of eigenstates

Consider a system with the following eigenstates.

$\lvert 0\rangle = (1\ 0\ 0\ 0)^\dagger$	no electrons
$\lvert 1\rangle = (0\ 1\ 0\ 0)^\dagger$	one electron in state ϕ_1
$\lvert 2\rangle = (0\ 0\ 1\ 0)^\dagger$	one electron in state ϕ_2
$\lvert 3\rangle = (0\ 0\ 0\ 1)^\dagger$	two electrons, one in state ϕ_1, one in state ϕ_2

Then for the wavefunction basis

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

and for $L = 10^{-9}$ meters we have

$$\hat{E} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.38\,\mathrm{eV} & 0 & 0 \\ 0 & 0 & 1.50\,\mathrm{eV} & 0 \\ 0 & 0 & 0 & 6.55\,\mathrm{eV} \end{pmatrix}$$

Let $\lvert\xi\rangle$ be the state vector

$$\lvert\xi\rangle = \frac{1}{2}\lvert 0\rangle + \frac{1}{2}\lvert 1\rangle + \frac{1}{2}\lvert 2\rangle + \frac{1}{2}\lvert 3\rangle = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$$

The expected energy is

$$\langle\xi\lvert\hat{E}\rvert\xi\rangle = \frac{0\,\mathrm{eV}}{4} + \frac{0.38\,\mathrm{eV}}{4} + \frac{1.50\,\mathrm{eV}}{4} + \frac{6.55\,\mathrm{eV}}{4} = 2.11\,\mathrm{eV}$$

For the system we are considering, the result of a single measurement is either 0 eV, 0.38 eV, 1.50 eV, or 6.55 eV. The value 2.11 eV is the expected average across multiple measurements. Recall that a measurement causes the system to exit state $\lvert\xi\rangle$ and enter an eigenstate $\lvert 0\rangle$, $\lvert 1\rangle$, $\lvert 2\rangle$, or $\lvert 3\rangle$ corresponding to the measured eigenvalue. The system must be put back in state $\lvert\xi\rangle$ before the next measurement.

To use a slot machine analogy, state $\lvert\xi\rangle$ is like the wheels spinning. Observing the system makes the wheels stop. The stopped wheels are in an eigenstate $\lvert 0\rangle$, $\lvert 1\rangle$, $\lvert 2\rangle$, or $\lvert 3\rangle$. Once they are stopped the wheels don't change, they remain in the same eigenstate. You have to pull the lever to get the wheels spinning again.