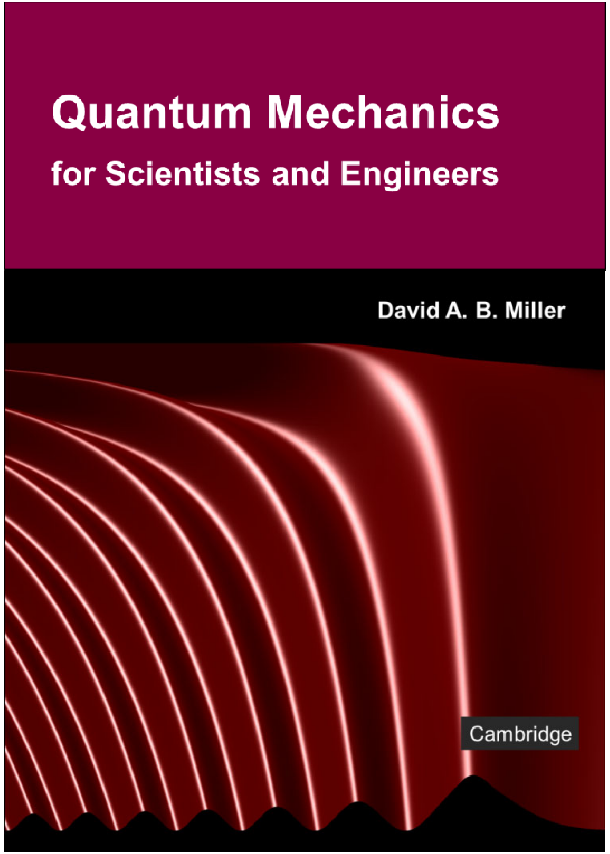
44 Fermion operators and multiple particles

Slides: Lecture 44a Single-particle fermion operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 16.3 subsection "Representation of general single-particle fermion operators"



Fermion operators and multiple particles

Single-particle fermion operators

Quantum mechanics for scientists and engineers

David Miller

General single-particle fermion operators

Here we consider a system with N fermions

In the $\mathbf{r}$ representation of an operator $\hat{G}_{\mathbf{r}}$

e.g., such as the momentum operator

for a multiple fermion system

we would add all of the operators

corresponding to the coordinates of each

particle, i.e.,

$$\hat{G}_{\mathbf{r}} = \sum_{i=1}^{N} \hat{G}_{\mathbf{r}i}$$

where $\hat{G}_{\mathbf{r}i}$ is the operator for a specific particle

e.g., it might be the momentum operator

General single-particle fermion operators

In the annihilation and creation operator formalism

we postulate instead that

$$\hat{G} = \int \hat{\psi}^{\dagger} \hat{G}_{\mathbf{r}} \hat{\psi} \, d^3\mathbf{r}_1 d^3\mathbf{r}_2 \ldots d^3\mathbf{r}_N$$

where

$$\hat{\psi}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\right) = \frac{1}{\sqrt{N}} \sum_{a,b,\ldots,n} \hat{b}_n \ldots \hat{b}_b \hat{b}_a \phi_a\left(\mathbf{r}_1\right) \phi_b\left(\mathbf{r}_2\right) \ldots \phi_n\left(\mathbf{r}_N\right)$$

is the N-particle fermion wavefunction operator, so

$$\hat{G} = \frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{a,b,\ldots n \\ a',b',\ldots n'}} \hat{b}_{a'}^{\dagger} \hat{b}_{b'}^{\dagger} \ldots \hat{b}_{n'}^{\dagger} \hat{b}_n \ldots \hat{b}_b \hat{b}_a$$

$$\times \int \phi_{a'}^*\left(\mathbf{r}_1\right) \phi_{b'}^*\left(\mathbf{r}_2\right) \ldots \phi_{n'}^*\left(\mathbf{r}_N\right) \hat{G}_{\mathbf{r}i} \phi_a\left(\mathbf{r}_1\right) \phi_b\left(\mathbf{r}_2\right) \ldots \phi_n\left(\mathbf{r}_N\right) d^3\mathbf{r}_1 d^3\mathbf{r}_2 \ldots d^3\mathbf{r}_N$$

General single-particle fermion operators

In

$$\hat{G} = \frac{1}{N}\sum_{i=1}^{N} \sum_{\substack{a,b,\ldots n \\ a',b',\ldots n'}} \hat{b}_{a'}^{\dagger}\hat{b}_{b'}^{\dagger}\ldots\hat{b}_{n'}^{\dagger}\hat{b}_{n}\ldots\hat{b}_{b}\hat{b}_{a}$$

$$\times\int \phi_{a'}^{*}(\mathbf{r}_1)\phi_{b'}^{*}(\mathbf{r}_2)\ldots\phi_{n'}^{*}(\mathbf{r}_N)\hat{G}_{\mathbf{r}i}\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2)\ldots\phi_n(\mathbf{r}_N)\,d^3\mathbf{r}_1 d^3\mathbf{r}_2\ldots d^3\mathbf{r}_N$$

each of the a, b, ..., n and each of the a', b', ..., n'

ranges over all single-particle fermion states

Now, all the spatial integrals, except the one over r_i

lead to Kronecker deltas of the form $\delta_{k'k}$

forcing $a' = a$, $b' = b$, etc., except for particle i

General single-particle fermion operators

Hence $\hat{G} = \frac{1}{N}\sum_{i=1}^{N}\sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\hat{b}_a^\dagger\hat{b}_b^\dagger\ldots\hat{b}_{i1}^\dagger\ldots\hat{b}_n^\dagger\hat{b}_n\ldots\hat{b}_{i2}\ldots\hat{b}_b\hat{b}_a$

where $G_{i1i2} = \int\phi_{i1}^*(\mathbf{r}_i)\hat{G}_{\mathbf{r}i}\phi_{i2}(\mathbf{r}_i)d^3\mathbf{r}_i$

We can use the anticommutation relation $\hat{b}_j\hat{b}_k + \hat{b}_k\hat{b}_j = 0$

to progressively swap the operator $\hat{b}_{i2}$

from the right to the center

and the anticommutation relation $\hat{b}_j^\dagger\hat{b}_k^\dagger + \hat{b}_k^\dagger\hat{b}_j^\dagger = 0$

to progressively swap the operator $\hat{b}_{i1}^\dagger$

from the left to the center

General single-particle fermion operators

Each such application of an anticommutation relation results in a sign change

but there are equal number of swaps from the left and from the right

so there is no net sign change in this operation

Hence we have

$$\hat{G} = \frac{1}{N} \sum_{i=1}^{N} \sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2} \underbrace{\hat{b}_a^\dagger \hat{b}_b^\dagger \ldots \hat{b}_n^\dagger}_{\text{omitting } \hat{b}_{i1}^\dagger} \hat{b}_{i1}^\dagger \hat{b}_{i2} \underbrace{\hat{b}_n \ldots \hat{b}_b \hat{b}_a}_{\text{omitting } \hat{b}_{i2}}$$

General single-particle fermion operators

In practice with any operator

in the end we are working out its matrix elements

Any two operators with identical matrix elements are equivalent operators

We consider two, possibly different, *N*-fermion basis states

$\left|\psi_{1N}\right\rangle$ and $\left|\psi_{2N}\right\rangle$

and consider matrix elements of the operator $\hat{G}$ in

$$\hat{G} = \frac{1}{N}\sum_{i=1}^{N}\sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\underbrace{\hat{b}_a^\dagger\hat{b}_b^\dagger\ldots\hat{b}_n^\dagger}_{\text{omitting } \hat{b}_{i1}^\dagger}\hat{b}_{i1}^\dagger\hat{b}_{i2}\underbrace{\hat{b}_n\ldots\hat{b}_b\hat{b}_a}_{\text{omitting } \hat{b}_{i2}}$$

between such states

General single-particle fermion operators

Because of Pauli exclusion

the only strings of operators that can survive in matrix elements for legal fermion states

are those in which the operators $\hat{b}_a, \hat{b}_b, \ldots \hat{b}_n$

are all different from each other

i.e., correspond to annihilation operators for different single particle states

and are each different from both $\hat{b}_{i1}$ and $\hat{b}_{i2}$

since otherwise we would be trying either to

annihilate two fermions from the same state or

create two fermions in the same state

General single-particle fermion operators

Hence, for these states

since no two states in the string of creation operators or in the string of annihilation operators can be identical

not only do the pairs of annihilation operators anticommute and

the pairs of creation operators anticommute as usual

so also do all the pairs of creation and annihilation operators with different subscripts

other than possibly the pair $\hat{b}_{i1}^{\dagger}\hat{b}_{i2}$

General single-particle fermion operators

Hence in $\hat{G} = \frac{1}{N} \sum_{i=1}^{N} \sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2} \underbrace{\hat{b}_a^\dagger \hat{b}_b^\dagger \ldots \hat{b}_n^\dagger}_{omitting\ \hat{b}_{i1}^\dagger} \hat{b}_{i1}^\dagger \hat{b}_{i2} \underbrace{\hat{b}_n \ldots \hat{b}_b \hat{b}_a}_{omitting\ \hat{b}_{i2}}$

we can swap the creation operator $\hat{b}_a^\dagger$

all the way from the left

until we get to the left of the corresponding

annihilation operator $\hat{b}_a$

only acquiring minus signs as we do so

General single-particle fermion operators

Actually, we acquire an even number of minus signs

because the number of swaps taken to get to the middle

is equal to

the number to get from the middle to its final position

so there is no change in sign in all these swaps

We can repeat this procedure for each creation operator

other than $\hat{b}_{i1}^{\dagger}$

which we do not need to move anyway

General single-particle fermion operators

Hence, with all these swaps, we can rewrite

$$\hat{G} = \frac{1}{N}\sum_{i=1}^{N}\sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\underbrace{\hat{b}_a^\dagger\hat{b}_b^\dagger\ldots\hat{b}_n^\dagger}_{\text{omitting }\hat{b}_{i1}^\dagger}\hat{b}_{i1}^\dagger\hat{b}_{i2}\underbrace{\hat{b}_n\ldots\hat{b}_b\hat{b}_a}_{\text{omitting }\hat{b}_{i2}}$$

as

$$\hat{G} = \frac{1}{N}\sum_{i=1}^{N}\sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\hat{b}_{i1}^\dagger\hat{b}_{i2}\underbrace{\hat{b}_n^\dagger\hat{b}_n\ldots\hat{b}_b^\dagger\hat{b}_b\hat{b}_a^\dagger\hat{b}_a}_{\text{omitting }\hat{b}_{i1}^\dagger\hat{b}_{i2}}$$

or more simply

$$\hat{G} = \frac{1}{N}\sum_{i=1}^{N}\sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\hat{b}_{i1}^\dagger\hat{b}_{i2}\underbrace{\hat{N}_n\ldots\hat{N}_b\hat{N}_a}_{\text{omitting }\hat{b}_{i1}^\dagger\hat{b}_{i2}}$$

General single-particle fermion operators

When this operator $\hat{G} = \frac{1}{N}\sum_{i=1}^{N} \sum_{a,b,\ldots,i1,i2,\ldots n} G_{i1i2}\hat{b}_{i1}^{\dagger}\hat{b}_{i2} \underbrace{\hat{N}_n \ldots \hat{N}_b \hat{N}_a}_{\text{omitting } \hat{b}_{i1}^{\dagger}\hat{b}_{i2}}$

operates on a specific N-fermion basis state $|\psi_{1N}\rangle$

the only terms in the summation that can survive

are those for which the list of states $a,b,\ldots n$

corresponds to occupied states in $|\psi_{1N}\rangle$

and so the sum over a, b, ..., n (omitting $i1$ and $i2$)

and the number operators

can be dropped without changing any matrix element

General single-particle fermion operators

Hence we can write $\hat{G} = \frac{1}{N} \sum_{i=1}^{N} \sum_{i1,i2} G_{i1i2} \hat{b}_{i1}^{\dagger} \hat{b}_{i2}$

It makes no difference which fermion we are considering

G_{i1i2} is the same for every fermion

so the sum over i is trivial, and so

$$\hat{G} = \sum_{j,k} G_{jk} \hat{b}_{j}^{\dagger} \hat{b}_{k}$$

where we also further simplified notation by substituting j for $i1$ and k for $i2$

General single-particle fermion operators

This is the general form for a single-particle fermion operator

$$\hat{G} = \sum_{j,k} G_{jk} \hat{b}_j^\dagger \hat{b}_k$$

The Hamiltonian

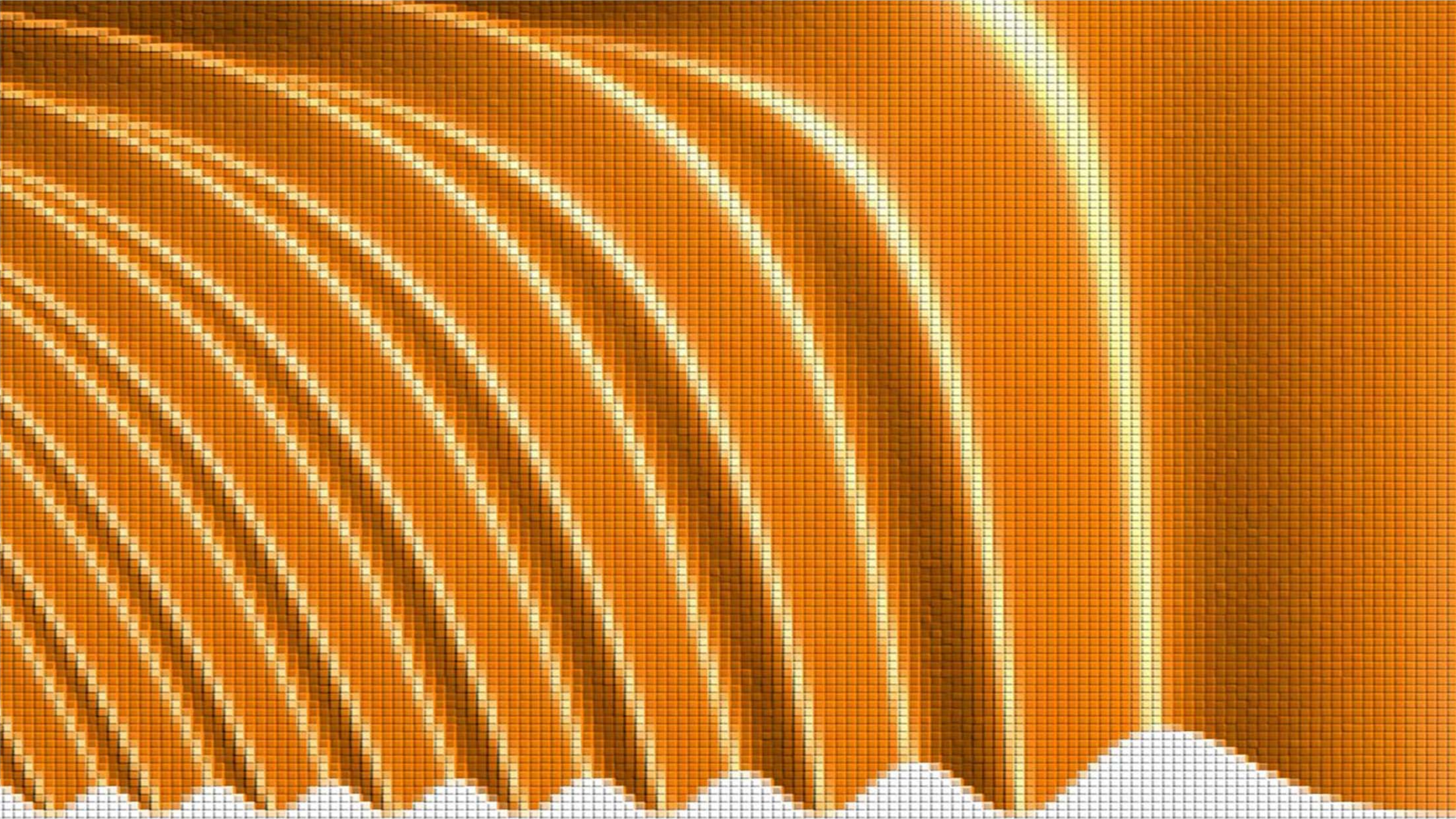
$$\hat{H} = \sum_j E_j \hat{b}_j^\dagger \hat{b}_j$$

is just a special case for a diagonal operator

Hence we have found a very simple form

for the single-particle fermion operator

valid for any number of fermions

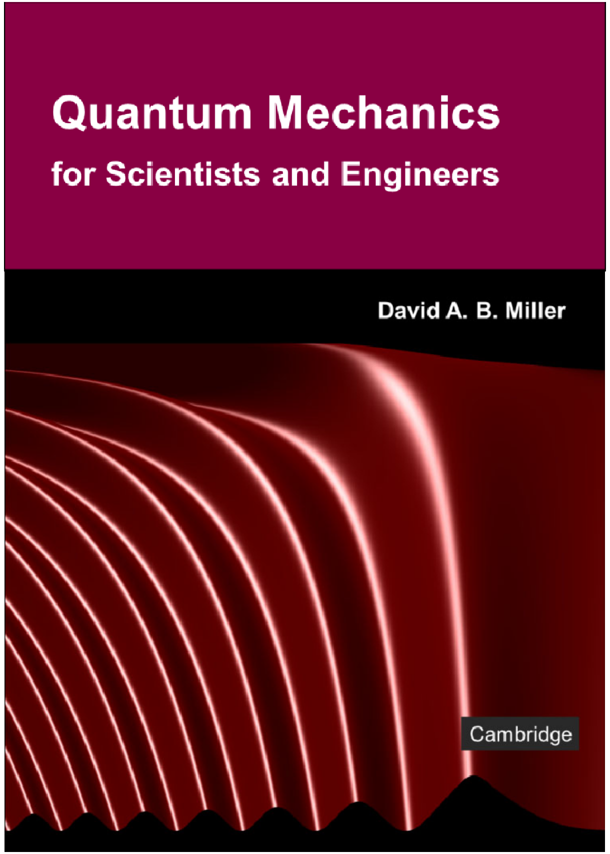


44 Fermion operators and multiple particles

Slides: Lecture 44b Two-particle fermion operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 16.3 subsection "Two-particle fermion operators"



Fermion operators and multiple particles

Two-particle fermion operators

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Two-particle fermion operators

Fermions such as electrons interact

e.g., through their Coulomb repulsion

For such cases, we need two-particle operators

In the $\mathbf{r}$ form, we might have an operator $\hat{D}_{\mathbf{r}}\left(\mathbf{r}_1,\mathbf{r}_2\right)$

that depends on the coordinates of both particles

Then we postulate we can write

$$\hat{D}=\int\hat{\psi}^{\dagger}\left(\mathbf{r}_1,\mathbf{r}_2\right)\hat{D}_{\mathbf{r}}\left(\mathbf{r}_1,\mathbf{r}_2\right)\hat{\psi}\left(\mathbf{r}_1,\mathbf{r}_2\right)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

using the two-fermion wavefunction operator

$$\hat{\psi}\left(\mathbf{r}_1,\mathbf{r}_2\right)=\frac{1}{\sqrt{2}}\sum_{j,k}\hat{b}_k\hat{b}_j\phi_j\left(\mathbf{r}_1\right)\phi_k\left(\mathbf{r}_2\right)$$

Two-particle fermion operators

Substituting this two-particle wavefunction operator

into $\hat{D} = \int \hat{\psi}^\dagger(\mathbf{r}_1, \mathbf{r}_2)\hat{D}_\mathbf{r}(\mathbf{r}_1, \mathbf{r}_2)\hat{\psi}(\mathbf{r}_1, \mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2$

we have

$$\hat{D} = \frac{1}{2}\sum_{a,b,c,d} \hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c \int \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)\hat{D}_\mathbf{r}(\mathbf{r}_1, \mathbf{r}_2)\phi_c(\mathbf{r}_1)\phi_d(\mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

or equivalently

$$\hat{D} = \frac{1}{2}\sum_{a,b,c,d} D_{abcd}\hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c$$

where

$$D_{abcd} = \int \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)\hat{D}_\mathbf{r}(\mathbf{r}_1, \mathbf{r}_2)\phi_c(\mathbf{r}_1)\phi_d(\mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

Order of suffixes in two-particle fermion operators

Note in

$$\hat{D} = \frac{1}{2} \sum_{a,b,c,d} D_{abcd} \hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c$$

the order of the suffixes on the chain of operators

$\hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c$ is not a, b, c, d

The ordering is in the opposite sense for the annihilation operators

This different ordering emerges

from the wavefunction operators

and the properties of Hermitian conjugation

Two-particle operators with multiple particles

We presume that the two-particle fermion operator

$$\hat{D} = \frac{1}{2} \sum_{a,b,c,d} D_{abcd} \hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c$$

would remain unchanged as we changed the system

to have more than two fermions in it

The arguments would be similar to those for the single-particle fermion operator $\hat{G} = \sum_{j,k} G_{jk} \hat{b}_j^\dagger \hat{b}_k$

So we presume this is a general statement

for a two-particle fermion operator

in this annihilation and creation operator approach

Electrons interacting through the Coulomb potential

For two electrons (of the same spin) with Coulomb repulsion

the Hamiltonian in the $\mathbf{r}$ form is

$$\hat{H}_{\mathbf{r}}\left(\mathbf{r}_1,\mathbf{r}_2\right) = -\frac{\hbar^2}{2m_o}\left(\nabla_{\mathbf{r}_1}^2 + \nabla_{\mathbf{r}_2}^2\right) + \frac{e^2}{4\pi\varepsilon_o\left|\mathbf{r}_1 - \mathbf{r}_2\right|}$$

Hence our two particle operator formalism gives us

$$\hat{H} = \frac{1}{2}\sum_{a,b,c,d} H_{abcd}\hat{b}_a^\dagger\hat{b}_b^\dagger\hat{b}_d\hat{b}_c$$

where H_{abcd} is defined analogously to

$$D_{abcd} = \int \phi_a^*\left(\mathbf{r}_1\right)\phi_b^*\left(\mathbf{r}_2\right)\hat{D}_{\mathbf{r}}\left(\mathbf{r}_1,\mathbf{r}_2\right)\phi_c\left(\mathbf{r}_1\right)\phi_d\left(\mathbf{r}_2\right)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

Electrons interacting through the Coulomb potential

Suppose specifically we have the two-fermion state

where one electron is in the basis state $\phi_k(\mathbf{r})$

and the other is in the basis state $\phi_m(\mathbf{r})$

i.e., the two-particle state can be written

$$|\psi_{TP}\rangle = \hat{b}_k^\dagger \hat{b}_m^\dagger |0\rangle$$

We evaluate the expectation value of the energy

using the Hamiltonian $\hat{H} = \frac{1}{2} \sum_{a,b,c,d} H_{abcd} \hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c$

for this state, i.e.

$$\langle \psi_{TP} | \hat{H} | \psi_{TP} \rangle = \frac{1}{2} \langle 0 | \sum_{a,b,c,d} H_{abcd} \hat{b}_m \hat{b}_k \hat{b}_a^\dagger \hat{b}_b^\dagger \hat{b}_d \hat{b}_c \hat{b}_k^\dagger \hat{b}_m^\dagger |0\rangle$$

Electrons interacting through the Coulomb potential

Now

$$\langle 0|\hat{b}_m\hat{b}_k\hat{b}_a^\dagger\hat{b}_b^\dagger\hat{b}_d\hat{b}_c\hat{b}_k^\dagger\hat{b}_m^\dagger|0\rangle =$$

$$\delta_{ak}\delta_{bm}\delta_{ck}\delta_{dm}+\delta_{am}\delta_{bk}\delta_{cm}\delta_{dk}-\delta_{am}\delta_{bk}\delta_{ck}\delta_{dm}-\delta_{ak}\delta_{bm}\delta_{cm}\delta_{dk}$$

the proof of which is left as an exercise

Hence we have for the energy expectation value

$$\langle\psi_{TP}|\hat{H}|\psi_{TP}\rangle = \frac{1}{2}\langle 0|\sum_{a,b,c,d} H_{abcd}\hat{b}_m\hat{b}_k\hat{b}_a^\dagger\hat{b}_b^\dagger\hat{b}_d\hat{b}_c\hat{b}_k^\dagger\hat{b}_m^\dagger|0\rangle$$

$$= \frac{1}{2}\left(H_{kmkm}+H_{mkmk}-H_{mkkm}-H_{kmmk}\right)$$

Electrons interacting through the Coulomb potential

In $\langle \psi_{TP} | \hat{H} | \psi_{TP} \rangle = \frac{1}{2}\left(H_{kmkm} + H_{mkmk} - H_{mkkm} - H_{kmmk} \right)$

explicitly, we have

$$H_{kmkm} = H_{mkmk} = \int \phi_k^*(\mathbf{r}_1)\phi_m^*(\mathbf{r}_2)\hat{H}_{\mathbf{r}}\phi_k(\mathbf{r}_1)\phi_m(\mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

and

$$H_{kmmk} = H_{mkkm}^* = \int \phi_k^*(\mathbf{r}_1)\phi_m^*(\mathbf{r}_2)\hat{H}_{\mathbf{r}}\phi_m(\mathbf{r}_1)\phi_k(\mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

These are exactly the same terms as previously calculated using the $\mathbf{r}$ formalism

Electrons interacting through the Coulomb potential

Remember in $\langle \psi_{TP} | \hat{H} | \psi_{TP} \rangle = \frac{1}{2}\left(H_{kmkm} + H_{mkmk} - H_{mkkm} - H_{kmmk} \right)$

H_{kmkm} or equivalently $(1/2)(H_{kmkm} + H_{mkmk})$ is the sum of the kinetic energies for the two particles and the Coulomb potential energy for two electrons

so it is the energy we would calculate if the particles were not identical

$-(1/2)(H_{mkkm} + H_{kmmk})$ is the exchange energy

Hence this approach does reproduce the results of our previous $\mathbf{r}$ formalism