Many Body Quantum Mechanics II

Spin 1/2 Fermions The formalism for many fermion systems is very similar to that for bosons. The great physical difference between multi-boson and multi-fermion systems is taken care of by replacing commutation relations with anti-commutation relations. We are again interested in a non-relativistic system, where there is no massive particle creation or destruction. We introduce a field operator for spin 1/2 fermions as follows:

$$\hat{\Psi}(\vec{x},0) = \sum_{\vec{k},s} \frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{x})\chi_s a_{\vec{k}s}, \tag{1}$$

where the χ_s are the familiar two component spinors describing spin "up" and "down." They are given by

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Eq.(1) describes a field operator which is a two component spinor, just as the wave function for a spin 1/2 system would be. We may project on individual spin components as follows:

$$\hat{\Psi}_s \equiv \chi_s^\dagger \hat{\Psi} = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{x}) a_{\vec{k}s} \tag{2}$$

In Eq.(1), the operators $a_{\vec{k}s}$ are destruction operators for fermions with wave vector $\vec{k}$, and spin projection s. The fact that we are treating fermions is contained in the fact that the $a_{\vec{k}s}$ and $a^\dagger_{\vec{k}s}$ obey *anticommutation* relations,

$$\{a_{\vec{k}s}, a^\dagger_{\vec{k}'s'}\} = \delta_{\vec{k},\vec{k}'}\delta_{s,s'}, \quad \{a_{\vec{k}s}, a_{\vec{k}'s'}\} = 0, \quad \{a^\dagger_{\vec{k}s}, a^\dagger_{\vec{k}'s'}\} = 0. \tag{3}$$

A consequence of these anti-commutation relations is that every time a fermi operator is moved past another fermi operator, there is a minus sign. (There may of course be a non-operator term as well if the anti-commutator is non-zero.)

The general form of various physical operators expressed in terms of field operators is very similar to the boson case. For example, the free Hamiltonian is

$$\hat{H}_0 = \sum_{\vec{k},s} a^\dagger_{\vec{k},s} a_{\vec{k}'s} E_{\vec{k}}, \tag{4}$$

where

$$E_{\vec{k}} = \frac{(\hbar\vec{k})^2}{2m}.$$

Expressed in terms of field operators, we have

$$\hat{H}_0 = \int d\vec{x} \hat{\Psi}^\dagger(\vec{x})(-\frac{(\hbar\nabla)^2}{2m})\hat{\Psi}(\vec{x}). \tag{5}$$

The form of the operator $\hat{V}$, which represents the two body potential acting between pairs of particles is also very similar. We have

$$\hat{V} = \frac{1}{2}\int d\vec{1}d\vec{2}\hat{\Psi}^{\dagger}(\vec{2})\hat{\Psi}^{\dagger}(\vec{1})V(\vec{1}-\vec{2})\hat{\Psi}(\vec{1})\hat{\Psi}(\vec{2}) \tag{6}$$

$$= \frac{1}{2}\sum_{s_2,s_1}\int d\vec{1}d\vec{2}\hat{\Psi}^{\dagger}_{s_2}(\vec{2})\hat{\Psi}^{\dagger}_{s_1}(\vec{1})V(\vec{1}-\vec{2})\hat{\Psi}_{s_1}(\vec{1})\hat{\Psi}_{s_2}(\vec{2}),$$

where in the second form, the spin indices have been displayed explicitly. For the fermion case the order of operators in $\hat{V}$ must be maintained exactly as written in Eq.(6).

With the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ in hand, we can define the Heisenberg field operator,

$$\hat{\Psi}(\vec{x},t) = \exp(\frac{i\hat{H}t}{\hbar})\hat{\Psi}(\vec{x},t)\exp(\frac{-i\hat{H}t}{\hbar})\hat{\Psi}.$$

The equation of motion satisfied by $\hat{\Psi}(\vec{x},t)$ follows upon using the anti-commutation relations. We have

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\vec{x},t) = -\frac{(\hbar\nabla)^2}{2m}\hat{\Psi}(\vec{x},t) + \int d\vec{x'}\hat{\Psi}^{\dagger}(\vec{x'},t)\hat{\Psi}(\vec{x'},t)V(\vec{x'}-\vec{x})\hat{\Psi}(\vec{x},t), \tag{7}$$

which has the same form as the corresponding equation for bosons.

The equation giving the Schrödinger wave function from the many body state vector $|\Phi_N>$ is also of the same form as it was for the boson case;

$$\Psi_N(\vec{x_1},\vec{x_2},\ldots,\vec{x_N},t) = \frac{1}{\sqrt{N!}} < 0|\hat{\Psi}(\vec{x_1},t)\hat{\Psi}(\vec{x_2},t),\ldots,\hat{\Psi}(\vec{x_N},t)|\Phi_N > . \tag{8}$$

The wave function with explicit spins for each particle is obtained by using the field components with definite spin projections, defined above in Eq.(2). We have

$$\Psi_{N,s_1s_2\ldots s_N}(\vec{x_1},\vec{x_2},\ldots,\vec{x_N},t) = \frac{1}{\sqrt{N!}} < 0|\hat{\Psi}_{s_1}(\vec{x_1},t)\hat{\Psi}_{s_2}(\vec{x_2},t),\ldots,\hat{\Psi}_{s_N}(\vec{x_N},t)|\Phi_N > \tag{9}$$

The anti-commutators Eq.(3) give rise to the equal time anti-commutator,

$$\{\hat{\Psi}_s(\vec{x},0),\hat{\Psi}^{\dagger}_{s'}(\vec{x'},0)\} = \sum_{\vec{k},\vec{k'}}(\frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x}))(\frac{1}{\sqrt{V}}\exp(-i\vec{k'}\cdot\vec{x'}))\{a_{\vec{k}s},a^{\dagger}_{\vec{k'}s'}\}$$

$$= \delta_{s,s'}\sum_{\vec{k}}\frac{1}{V}\exp(i\vec{k}\cdot(\vec{x}-\vec{x'})) = \delta_{s,s'}\delta^3(\vec{x}-\vec{x'}).$$

The corrsponding equal time anti commutator involving $\hat{\Psi}(\vec{x},t)$ with itself vanishes as does the anti commutator involving $\hat{\Psi}^{\dagger}(\vec{x},t)$ with itself.

Scattering of Identical Fermions The present formalism is designed for a treatment of a large, uniform system of fermions. However, it is also useful in any problem involving more than one fermion. Whereas in dealing with the Schrödinger equation, antisymmetry must be done by hand, when the problem is formulated using the field operators defined in the previous section, antisymmetry is handled automatically. We illustrate for the case of scatttering of two identical spin 1/2 fermions. The method used here is a simple example of the treatment that is necessary in dealing with relativistic fermions using the Dirac equation and Feynman diagrams.

We start with the breakup of Hamiltonian into a free part and an interaction part.

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where $\hat{H}_0$ and $\hat{V}$ are given in Eqs.(5) and (6), respectively. The initial and final states

$$|i >= a^{\dagger}_{\vec{k}_1 s_1} a^{\dagger}_{\vec{k}_2 s_2}|0 >,$$

and

$$|f >= a^{\dagger}_{\vec{k'}_1 s'_1} a^{\dagger}_{\vec{k'}_2 s'_2}|0 >,$$

both of which represent two fermions in states of definite momenta and spin projection. The scattering process is governed by the $U(\infty, -\infty)$ operator. Recall that the interaction picture operator $U(t_2, t_1)$, governs the evolution of a state known at t_1 to its value at t_2. The matrix element of $U(\infty, -\infty)$ gives the probability amplitude for a state initially in $|i >$, to have evolved to $|f >$ at $t = \infty$. The perturbation expansion of $U(\infty, -\infty)$ is given by

$$< f|U(\infty, -\infty)|i >=< f|I - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt\hat{V}_I(t) + \ldots |i > .$$

All the operators in $\hat{V}$ are in the interaction picture. This means that the field operator $\hat{\Psi}(\vec{x}, t)$ satisfies the free Schrödinger equation. In terms of destruction operators, we have

$$\hat{\Psi}_I(\vec{x}, t) = \sum_{\vec{k},s} \frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{x} - i\omega_{\vec{k}}t) a_{\vec{k}s}\chi_s,$$

where as usual,

$$\hbar\omega_{\vec{k}} = E_{\vec{k}} = \frac{(\hbar\vec{k})^2}{2m}.$$

We will calculate the first order matrix element of $U(\infty, -\infty)$.

$$< f|U^1(\infty, -\infty)|i > -\frac{i}{\hbar} < f| \int_{-\infty}^{\infty} dt\hat{V}_I(t)|i >=$$

$$-\frac{i}{2\hbar}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d\vec{1}d\vec{2} < f|\hat{\Psi}^{\dagger}_I(\vec{2}, t)\hat{\Psi}^{\dagger}_I(\vec{1}, t)V(\vec{1} - \vec{2})\hat{\Psi}_I(\vec{1}, t)\hat{\Psi}_I(\vec{2}, t)|i >$$

Now imagine sandwiching the identity operator right after the $\hat{\Psi}_I(\vec{1},t)\hat{\Psi}_I(\vec{2},t)$ operators which act on the initial state, $|i>$. We may write

$$I = |0 >< 0| + \sum_{one} |1 >< 1| + \sum_{two} |2 >< 2| + \ldots ,$$

where $\sum_{one} |1 >< 1|$ represents the sum over all one particle states, and so on for more particles. It is easy to see that the only term out of the sum which contributes is $|0 >< 0|$. All terms in the operator product $\hat{\Psi}_I(\vec{1},t)\hat{\Psi}_I(\vec{2}t)$ contain two destruction operators. Either the $\vec{k}s$ indices of these operators match those in $|i>$, or they may move past the creation operators in $|i>$, but if they do so, they meet and destroy the vacuum $|0>$. Given this, we only need to evaluate

$$< 0|\hat{\Psi}_I(\vec{1},t)\hat{\Psi}_I(\vec{2},t)a^\dagger_{\vec{k}_1s_1}a^\dagger_{\vec{k}_2s_2}|0> .$$

Straightforward application of the anti-commutation rules gives the result;

$$(\frac{1}{\sqrt{V}}\exp(i\vec{k}_1\cdot\vec{x}_2 - i\omega_1 t)\chi_{s_1}(2))(\frac{1}{\sqrt{V}}\exp(i\vec{k}_2\cdot\vec{x}_1 - i\omega_2 t)\chi_{s_2}(1))$$

$$-(\frac{1}{\sqrt{V}}\exp(i\vec{k}_1\cdot\vec{x}_1 - i\omega_1 t)\chi_{s_1}(1))(\frac{1}{\sqrt{V}}\exp(i\vec{k}_2\cdot\vec{x}_2 - i\omega_2 t)\chi_{s_2}(2))$$

where

$$\hbar\omega_1 = \frac{(\hbar\vec{k}_1)^2}{2m},\ etc$$

The evaluation of

$$< f|\hat{\Psi}^\dagger(\vec{2}',t)\hat{\Psi}^\dagger(\vec{1}',t)|0>$$

is very similar. We put $\prime$ on all momenta and spin labels, take the complex conjugate of plane wave factors, and replace all χ column vectors by $\chi^\dagger$ row vectors. The resulting matrix element has four terms in it as shown in the Figure.

Now all the terms $(a)-(d)$ have the same time dependence. We can then do the time integral, obtaining

$$\int_{-\infty}^{\infty} dt \exp(it(\omega_1' + \omega_2' - \omega_1 - \omega_2)) = 2\pi\delta(\omega_1' + \omega_2' - \omega_1 - \omega_2),$$

which expresses overall energy conservation in the scattering process.

For doing the spacial integrals, we need to Fourier analyze the potential. Expanding $V(\vec{x}_1 - \vec{x}_2)$,

$$V(\vec{x}_1 - \vec{x}_2) = \frac{1}{V}\sum_{\vec{q}} \tilde{V}(\vec{q})\exp(i\vec{q}\cdot(\vec{x}_1 - \vec{x}_2))$$

By relabelling $\vec{x}_1$ and $\vec{x}_2$, we have that the contributions of diagrams (a) and (d) are equal. Likewise the contributions of diagrams (b) and (c) are equal. We may handle this by evaluating (a) and (b) and omitting the overall factor of $1/2$ in $\hat{V}$. Treating first the contribution of $(a)+(d)$, the spacial integral gives

$$\int d\vec{x}_1 d\vec{x}_2 \exp(-i\vec{k'}_2\cdot\vec{x}_1 - i\vec{k'}_1\cdot\vec{x}_2 + i\vec{k}_2\cdot\vec{x}_1 + i\vec{k}_2\cdot\vec{x}_1 + i\vec{q}\cdot(\vec{x}_1-\vec{x}_2))$$

$$= V\delta_{\vec{k'}_2-\vec{k}_2,\vec{q}}V\delta_{\vec{k}_1-\vec{k'}_1,\vec{q}}$$

Carrying out the sum on $\vec{q}$, we satisfy one of the Kronecker δ functions, leaving one which expresses overall momentum conservation. For $(a)+(d)$ we now have the expression

$$-\frac{i}{\hbar}2\pi\delta(\omega_1'+\omega_2'-\omega_1-\omega_2)V^2\delta_{\vec{k'}_1+\vec{k'}_2,\vec{k}_1+\vec{k}_2}(\frac{1}{\sqrt{V}})^4\frac{1}{V}\tilde{V}(\vec{k'}_2-\vec{k}_2)(\chi^\dagger_{s_2'}\chi_{s_2})(\chi^\dagger_{s_1'}\chi_{s_1})$$

We obtain the full answer by adding in the expression obtained by the interchange $\vec{k}_1, s_1 \leftrightarrow \vec{k}_2, s_2$. Our final expression for the first order matrix element of $U(\infty,-\infty)$ is

$$< f|U^1(\infty,-\infty)|i >= -\frac{i}{\hbar}2\pi\delta(\omega_1'+\omega_2'-\omega_1-\omega_2)V^2\delta_{\vec{k'}_1+\vec{k'}_2,\vec{k}_1+\vec{k}_2}(\frac{1}{\sqrt{V}})^4\frac{1}{V}\mathcal{M}_{fi},$$

where

$$\mathcal{M}_{fi} = \tilde{V}(\vec{k'}_2-\vec{k}_2)(\chi^\dagger_{s_2'}\chi_{s_2})(\chi^\dagger_{s_1'}\chi_{s_1}) - \tilde{V}(\vec{k'}_2-\vec{k}_1)(\chi^\dagger_{s_2'}\chi_{s_1})(\chi^\dagger_{s_1'}\chi_{s_2}).$$

Note that both terms involve the Fourier transform of the potential. The expression for $\mathcal{M}_{fi}$ can easily be written down from a glance at the diagrams in the Figure.

Transition Rate and Crossection The final step in the calculation is to turn the matrix element of $U(\infty,-\infty)$ into the physically accessible quantity, the scattering crossection. Our first move is to get the transition rate, i.e. the number of transitions/sec. For this we apply the usual Fermi method,which involves stripping off the energy conservation δ function, including the factor of 2π, squaring the rest, replacing the energy δ function times 2π, and summing over final states of the system. This gives

$$\mathcal{R} = \sum_f 2\pi\delta(\omega_1'+\omega_2'-\omega_1-\omega_2)V^4\delta_{\vec{k'}_1+\vec{k'}_2,\vec{k}_1+\vec{k}_2}(\frac{1}{V})^4\frac{1}{V^2}|\frac{1}{\hbar}\mathcal{M}_{fi}|^2.$$

Note that the square of a Kronecker δ is again a Kronecker δ. Next, we want to take the infinite volume limit. Converting the Kronecker δ to a Dirac δ function is done by

$$V\delta_{\vec{k'}_1+\vec{k'}_2,\vec{k}_1+\vec{k}_2} \rightarrow (2\pi)^3\delta^3(\vec{k'}_1+\vec{k'}_2-\vec{k}_1-\vec{k}_2)$$

The sum on discrete final wave vectors becomes an integral in the infinite volume limit, so the sum over final state becomes

$$\sum_f = \sum_{s_2'}\frac{V}{(2\pi)^3}\int d\vec{k'}_2\sum_{s_1'}\frac{V}{(2\pi)^3}\int d\vec{k'}_1$$

For a two particle collision, the point at which the particles interact can be anywhere in the volume V. This implies that the quantity of interest is not the transition rate $\mathcal{R}$, but rather $\mathcal{R}/V$, the number of transitions/volume/sec. Finally, as in all scattering problems, we must divide by the so-called "incident flux," which is a measure of how many particles are actually colliding. In our problem we have two initial particles, each contained in V, so the incident flux $\mathcal{F}$ is defined by

$$\mathcal{F} = \frac{|\vec{v}_1 - \vec{v}_2|}{V^2}, \quad \vec{v}_1 = \frac{1}{m}\hbar\vec{k}_1, \ etc$$

The desired physical quantity, the scattering crossection, is obtained by dividing the number of transitions/volume/sec by the incident flux, or

$$\sigma = \frac{1}{\mathcal{F}}(\frac{\mathcal{R}}{V})$$

Using our matrix elements, we finally have

$$\sigma = \frac{1}{|\vec{v}_1 - \vec{v}_2|} \sum_{s'_2,s'_1} \int \frac{d\vec{k'}_2}{(2\pi)^3} \int \frac{d\vec{k'}_1}{(2\pi)^3} (2\pi)^4 \delta(\omega_f - \omega_i) \delta^3(\vec{k}_f - \vec{k}_i) |\frac{1}{\hbar}\mathcal{M}_{fi}|^2,$$

where

$$\omega_f = \omega'_2 + \omega'_1, \quad \omega_i = \omega_2 + \omega_1, \quad \vec{k}_f = \vec{k'}_2 + \vec{k'}_1, \quad \vec{k}_i = \vec{k}_2 + \vec{k}_1$$

Spin Sums It often happens that final spins are not observed, so it is useful to have a formula for the case where all final spins are accepted. Suppose the matrix element for a final spin s' is of the form

$$\chi^\dagger A$$

where A is a two component column vector. Any physical quantity will involve the *square* of the matrix element,

$$A^\dagger \chi_{s'} \chi^\dagger_{s'} A.$$

Now if we are summing on final spins s', we will have

$$\sum_{s'} \chi_{s'} \chi^\dagger_{s'} = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

This makes the sum on final spins very easy. We have

$$\sum_{s'} A^\dagger \chi_{s'} \chi^\dagger_{s'} A = A^\dagger A$$

Averaging over an initial spin is also straightforward, but since an average is being taken, we divide by 2 for each spin being averaged.

Figure 1: Feynman diagrams for identical fermion scattering