Many Body Quantum Mechanics

In this section, we set up the many body formalism for quantum systems. This is useful in any problem involving identical particles. For example, it automatically takes care of "statistics" in identical particle scattering. It is also useful for treating large, uniform systems of identical particles. The most studied case for bosons is a gas or liquid of He^4 atoms. For fermions, there are several interesting systems, the electron "gas", nuclear matter, He^3, etc. In all cases treated here, the particles move non-relativistically, and interact through a potential. There is no creation or destruction of massive particles. Of course our systems can be coupled to photons, and photon creation and destruction is then certainly allowed. Most of our treatment will concern the system of massive bosons or fermions interacting through a potential.

Bosons We start by considering a set of spinless bosons in a box of volume V. Without obvious motivation at present, we introduce a set of creation and destruction operators satisfying the following commutation rules.

$$[a_{\vec{k}}, a^{\dagger}_{\vec{k'}}] = \delta_{\vec{k},\vec{k'}}$$

In addition, we assume

$$[a^{\dagger}_{\vec{k}}, a^{\dagger}_{\vec{k'}}] = [a_{\vec{k}}, a_{\vec{k'}}] = 0. \quad (1)$$

In these equations, the $\vec{k}$ and $\vec{k'}$ are the usual wave vectors for a particle in a box. Using these operators, we can now build up a many-particle space, or "Fock" space. This step is rather analogous to what we have done for photons, except here there is no spin or polarization. We have various sectors containing definite numbers of particles:

$$|0> \quad \text{no particle state},$$

or for one particle, we act with one creation operator,

$$a^{\dagger}_{\vec{k}}|0> \quad \text{one particle state}.$$

The ordinary quantum mechanical wave function for such a one particle state is

$$\frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{x}).$$

Two particle states are then

$$a^{\dagger}_{\vec{k}} a^{\dagger}_{\vec{k'}}|0> \quad \text{two particle state}.$$

Checking the normalization by use of the commutation rules, we have

$$< 0|a_{\vec{k'}} a_{\vec{k}} a^{\dagger}_{\vec{k}} a^{\dagger}_{\vec{k'}}|0 >$$

$$=< 0|a_{\vec{k'}}a^\dagger_{\vec{k'}}|0> + < 0|a_{\vec{k'}}a^\dagger_{\vec{k}}a_{\vec{k}}a^\dagger_{\vec{k'}}|0>$$
$$= 1 + < 0|a_{\vec{k'}}a^\dagger_{\vec{k}}a^\dagger_{\vec{k'}}a_{\vec{k}}|0>$$
$$= 1, \quad (\vec{k} \neq \vec{k'}),$$

so our state is normalized. We are discussing bosons, so the quantum mechanical two body wave function would be

$$\Psi(\vec{x},\vec{x'}) = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x})\frac{1}{\sqrt{V}}\exp(i\vec{k'}\cdot\vec{x'}) + \frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x'})\frac{1}{\sqrt{V}}\exp(i\vec{k'}\cdot\vec{x})\right).$$

For bosons, there is nothing to forbid two particles being in the same state. For this case, the normed state would be

$$\frac{1}{\sqrt{2}}a^\dagger_{\vec{k}}a^\dagger_{\vec{k}}|0>,$$

with corresponding wave function,

$$\Psi(\vec{x},\vec{x'}) = \frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x})\frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x'}). \quad (2)$$

It is clear from Eq.(1) that a two body state constructed by applying say N creation operators to $|0>$, will be symmetric under interchange of their *wave vectors.* This makes it clear we have a set of bosons. The wave function for such a state is of course also symmetric under interchange of particle *coordinates.* So we seem to have two parallel descriptions. They are easy to relate once we introduce a *field operator.* This is defined by

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

where all operators which act in the many particle or Fock space have ˆ symbols placed above them.

For a one-particle state, the wave function is a matrix element involving one field operator,

$$< 0|\hat{\Psi}(\vec{x})a^\dagger_{\vec{k}}|0> = \frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{x}).$$

This follows directly upon moving the $\hat{\Psi}$ operator to the right and using the commutation rule Eq.(1). For a two particle state, two field operators are needed,

$$\frac{1}{\sqrt{2}} < 0|\hat{\Psi}(\vec{x})\hat{\Psi}(\vec{x'})a^\dagger_{\vec{k}}a^\dagger_{\vec{k'}}|0> = \Psi_2(\vec{x},\vec{x'})$$

In general, suppose $|\Phi_N>$ is the state vector in the many body space, with normalization

$$< \Phi_N|\Phi_N> = 1.$$

Then the N body Schrödinger wave function is

$$\Psi_N(\vec{x_1},\vec{x_2},\ldots,\vec{x_N}) = \frac{1}{\sqrt{N!}} < 0|\hat{\Psi}(\vec{x_1})\hat{\Psi}(\vec{x_2}),\ldots,\hat{\Psi}(\vec{x_N})|\Phi_N> \quad (3)$$

Operators Any quantum mechanical operator which can be defined for a many particle system must be able to be represented in terms of creation and destruction operators, or equivalently, field operators. A simple operator is the number of particles. Writing it directly in terms of creation and destruction operators, we have

$$\hat{N} = \sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}}.$$

This can be represented in terms of field operators by

$$\hat{N} = \int d\vec{x} \hat{\Psi}^{\dagger}(\vec{x}) \hat{\Psi}(\vec{x}).$$

Likewise the free Hamiltonian is

$$\hat{H}_0 = \sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}} E_{\vec{k}}, \tag{4}$$

where

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

The field operator representation is

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

These formulas follow directly from the fact that we expanded the field operator in a complete set of orthogonal functions.

Free Schrödinger Equation For free particles, we use $\hat{H}_0$ to make the field operators move in time. We define

$$\hat{\Psi}(\vec{x}, t) = \exp(\frac{i}{\hbar} \hat{H}_0 t) \hat{\Psi}(\vec{x}, 0) \exp(\frac{-i}{\hbar} \hat{H}_0 t). \tag{5}$$

Using Eqs.(1) and (4) to compute the commutator, we have

$$[\hat{\Psi}(\vec{x}, 0), \hat{H}_0] = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \exp(i\vec{k} \cdot \vec{x}) E_{\vec{k}} a_{\vec{k}} = -\frac{(\hbar \nabla)^2}{2m} \hat{\Psi}(\vec{x}, 0).$$

Along with the definition Eq.(5), this implies

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\vec{x}, t) = -\frac{(\hbar \nabla)^2}{2m} \hat{\Psi}(\vec{x}, t).$$

This resembles the free Schrödinger equation for one particle in ordinary quantum mechanics, but since $\hat{\Psi}$ is an operator, it actually describes the free Schrödinger equation for any number of particles.

The Potential and the Interacting Schrödinger Equation A useful formula which is equivalent to Eq.(1) is the equal time commutator of $\hat{\Psi}$ with $\hat{\Psi}^\dagger$. Directly using Eq.(1), we have

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

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

Now we introduce an operator which represents the interaction between particles due to a two-body potential. We define

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

In Eq.(6), we have used a streamlined notation, $\vec{1} = \vec{x_1}$, etc. All operators are at a common time. The full Hamiltonian is now

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

Since energy is conserved, $\hat{H}$ is independent of time, so the field operators in $\hat{H}$ can be evaluated at time t or 0 or any other convenient value. With $\hat{H}$ in hand, we define the full Heisenberg field operator

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

Taking the time derivative will give us the full equation of motion for $\hat{\Psi}(\vec{x},t)$. We have

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\vec{x},t) = \exp(\frac{i\hat{H}t}{\hbar})[\hat{\Psi}(\vec{x},0),\hat{H}]\exp(\frac{-i\hat{H}t}{\hbar})\hat{\Psi} \tag{7}$$

$$= -\frac{(\hbar\nabla)^2}{2m}\hat{\Psi}(\vec{x},t) + \exp(\frac{i\hat{H}t}{\hbar})[\hat{\Psi}(\vec{x},0),\hat{V}]\exp(\frac{-i\hat{H}t}{\hbar})\hat{\Psi}$$

The first term on the right hand side of Eq.(7) follows from our previous results on the free Schrödinger equation. The commutator involving $\hat{V}$ is

$$[\hat{\Psi}(\vec{x},0),\hat{V}] = \frac{1}{2}\int d\vec{x_1}d\vec{x_2}[\delta^3(\vec{x}-\vec{x_2})\hat{\Psi}^\dagger(\vec{x_1},0)\hat{\Psi}(\vec{x_1},0)\hat{\Psi}(\vec{x_2},0)$$

$$+\hat{\Psi}^\dagger(\vec{x_2},0)\delta^3(\vec{x}-\vec{x_1},0)\hat{\Psi}(\vec{x_1},0)\hat{\Psi}(\vec{x_2},0)]V(\vec{x_1}-\vec{x_2})$$

$$= \int d\vec{x'}\hat{\Psi}^\dagger(\vec{x'},0)\hat{\Psi}(\vec{x'},0)V(\vec{x'}-\vec{x})\hat{\Psi}(\vec{x},0).$$

The exponentials involving $\hat{H}t/\hbar$ will convert all operators at time 0 to time t. We finally have the full Heisenberg equation of motion for $\hat{\Psi}(\vec{x},t)$,

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\vec{x},t) = -\frac{(\hbar\nabla)^2}{2m}\hat{\Psi}(\vec{x},t) + \int d\vec{x'}\hat{\Psi}^\dagger(\vec{x'},t)\hat{\Psi}(\vec{x'},t)V(\vec{x'}-\vec{x})\hat{\Psi}(\vec{x},t) \tag{8}$$

Eq.(8) is easy to understand. The operator $\hat{\Psi}^\dagger(\vec{x'},t)\hat{\Psi}(\vec{x'},t)$ is the density of particles at $\vec{x'}$. The potential term can then be thought of as the interaction between the particles at $\vec{x'}$ with the particle at $\vec{x}$, integrated over all $\vec{x'}$.

Eq.(8 will reproduce the full N particle Schrödinger equation. Showing this involves using Eq.(3) with all the field operators at time t, and differentiating. We will illustrate for the case $N = 2$. Higher values of N use the same technique. We start with the 2 particle wave function,

$$\Psi_2(\vec{x}_1,\vec{x}_2,t) = \frac{1}{\sqrt{2}} < 0|\hat{\Psi}(\vec{x}_1,t)\hat{\Psi}(\vec{x}_1,t)|\Phi_2 >$$

Differentiating with respect to t we have

$$i\hbar\frac{\partial}{\partial t}\Psi_2(\vec{x}_1,\vec{x}_2,t) = \frac{1}{\sqrt{2}} < 0|[\hat{\Psi}(\vec{x}_1,t),\hat{H}]\hat{\Psi}(\vec{x}_2,t)|\Phi_2 > + \frac{1}{\sqrt{2}} < 0|\hat{\Psi}(\vec{x}_1,t)[\hat{\Psi}(\vec{x}_2,t),\hat{H}]|\Phi_2 >$$

The $\hat{H}_0$ terms in $\hat{H}$ just deliver the free Schrödinger operator on each field, so we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_2(\vec{x}_1,\vec{x}_2,t) &= -(\frac{(\hbar\nabla_1)^2}{2m} + \frac{(\hbar\nabla_2)^2}{2m})\Psi_2(\vec{x}_1,\vec{x}_2,t) \\ &+\frac{1}{\sqrt{2}}\int d\vec{x'} < 0|\hat{\Psi}^\dagger(\vec{x'},t)\hat{\Psi}(\vec{x'},t)\hat{\Psi}(\vec{x}_1,t)\hat{\Psi}(\vec{x}_2,t)|\Phi_2 > V(\vec{x'}-\vec{x}_1) \\ &+\frac{1}{\sqrt{2}}\int d\vec{x'} < 0|\hat{\Psi}(\vec{x}_1,t)\hat{\Psi}^\dagger(\vec{x'},t)\hat{\Psi}(\vec{x'},t)\hat{\Psi}(\vec{x}_2,t)|\Phi_2 > V(\vec{x'}-\vec{x}_2) \end{aligned}$$

The term in $V(\vec{x'}-\vec{x}_1)$ vanishes because it has three destruction operators acting on a two particle state. For the term in $V(\vec{x'}-\vec{x}_2)$, we move $\hat{\Psi}^\dagger(\vec{x'},t)$ to the left, and obtain

$$\frac{1}{\sqrt{2}}\int d\vec{x'} < 0|\delta^3(\vec{x'}-\vec{x}_1)\hat{\Psi}(\vec{x'},t)\hat{\Psi}(\vec{x}_2,t)|\Phi_2 > V(\vec{x'}-\vec{x}_2) = V(\vec{x}_1-\vec{x}_2)\Psi_2(\vec{x}_1,\vec{x}_2,t)$$

We finally have

$$i\hbar\frac{\partial}{\partial t}\Psi_2(\vec{x}_1,\vec{x}_2,t) = -(\frac{(\hbar\nabla_1)^2}{2m} + \frac{(\hbar\nabla_2)^2}{2m})\Psi_2(\vec{x}_1,\vec{x}_2,t) + V(\vec{x}_1-\vec{x}_2)\Psi_2(\vec{x}_1,\vec{x}_2,t),$$

which is the $N = 2$ Schrödinger equation. Cases of higher N are done in a similar manner.