Physics 555 Fall 2004 (instructor: P. B. Allen)
Notes on Creation and Destruction Operators

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The Schrödinger equation of the harmonic oscillator simplifies by introducing raising and lowering operators. The electromagnetic field in a cavity is mathematically equivalent to an infinite set of harmonic oscillators, one for each normal mode. The vibrations of a solid with Born-von Karman boundary conditions are also a set of harmonic oscillators, almost infinite in number, but actually numbering $3N$. In these "many-body" situations, algebra is simplified by raising and lowering operators, and additional simplification occurs by reinterpretation of these operators as creation and destruction operators for new particles (photons or phonons respectively). Their algebra is familiar from the elementary context in which they are introduced.

Superconductivity is a many electron problem for which the algebra of creation and destruction operators provides a very important simplification. Unfortunately, there is no elementary context analogous to the simple harmonic oscillator where these operators can be introduced. We have to go directly to the many electron problem and imagine processes in which the number of electrons is changing. This is not quite as natural as imagining the number of phonons changing since phonons have an alternate interpretation as the quantized excitations of an underlying system with a fixed number of atoms. It is good to forget this alternate interpretation of the lattice problem, and deal with phonons as real particles which can be created and destroyed. Electrons in solid state physics can not be created alone, but we can create simultaneously an electron and a hole. This just means that an electron is promoted out of a filled state into an empty state. The newly filled state is called an electron, and the newly vacated state is called a hole. We can use an alternate language in which the promotion process is described as destruction of an electron in the state which is being vacated, and simultaneous creation of an electron in the state which is being newly occupied. The algebra of these creation and destruction operators is very similar to the algebra of the corresponding operators for phonons, except that a minus sign pops up in various places which totally changes things and gives a wonderful way to deal with the antisymmetry of the many electron wavefunction.

In these notes I will not really derive the results at all, just list them. You can find them in many books. A place where the discussion appeals to me is Chapter 1 of *Quantum Theory of Finite Systems* by J.-P. Blaizot and G. Ripka (MIT Press, Cambridge, 1985).

For phonons, we start with normal mode eigenvectors and eigenfrequencies. These can be good approximate normal mode states for an actual solid which is nearly harmonic, or they could just be the eigenstates of an arbitrarily chosen Hamiltonian which has the same symmetries as the real system. Let the normal mode eigenstates be labeled with a quantum number i, where i runs from 1 to $3N$. Then a complete set of states for the vibrations of any real system with the same symmetries is

$$|n_1, n_2, \ldots, n_i, \ldots, n_{3N}> \tag{1}$$

where the integer n_1 is the occupancy of state 1 (the number of phonons in state 1), etc. These states span an infinite space known as the Fock space of the vibrational problem.

In a similar way we define the Fock space of the many electron problem. We need a complete orthonormal set of single electrons states $\psi_i(\vec{r})$. These states will often be chosen as the eigenstates of a single-particle Hamiltonian $\mathcal{H}_0$ which gives a first approximation to the properties of the actual many electron system. For example, they are very likely Bloch states where i is short for $(\vec{k}, n, \sigma)$. Or they may be free electron states $(\vec{k}, \sigma)$ where this time $\vec{k}$ is not restricted to the first Brillouin zone. The Fock space is spanned by the states

$$|n_1, n_2, \ldots, n_i, \ldots> \tag{2}$$

where the integer n_1 is again the occupancy of the electron state 1. Unlike phonons, the electron state is anti-symmetric in the coordinates of the various electrons. Not all the consequences of this are immediately clear, but one which is clear is that the occupancies n_i of electron states cannot be any non-negative integer, but are restricted to 0 or 1. Also, there are an infinite number of different electron states $\psi_i(\vec{r})$ in the list whose occupancy is to be specified, whereas for phonons there are only $3N$ classical eigenstates. Finally, unlike for phonons, the sum $\sum_i n_i = N$ is a conserved quantity, the number of electrons.

For phonons, the creation operator $a_i^\dagger$ is defined by the fact that it changes the many phonon state $|n_1, n_2, \ldots, n_i, \ldots, n_{3N}>$ into the state $(n_i+1)^{1/2}|n_1, n_2, \ldots, n_i+1, \ldots, n_{3N}>$. Exactly the same definition works for the electron creation operator $c_i^\dagger$. Now consider states formed by sequential operation of two different creation operators. For the phonon state $|\ldots, n_i+1, \ldots, n_j+1, \ldots, n_{3N}>$, it does not matter which operation occurred first. That is, the operators $a_i^\dagger a_j^\dagger$ and $a_j^\dagger a_i^\dagger$ do exactly the same thing to any state they operate on. Therefore the operators $a_i^\dagger$ and

$a_j^\dagger$ commute with each other. However, for electron states, adding two electrons to get $|\ldots, n_i+1, \ldots, n_j+1, \ldots>$ carries a permutation sign which depends on which state was added first. Thus $c_i^\dagger c_j^\dagger$ and $c_j^\dagger c_i^\dagger$ do the same thing except one is the negative of the other. This means that the operators $c_i^\dagger$ and $c_j^\dagger$ anticommute with each other.

Similar arguments show that the commutators $[a_i, a_j]$ and the anticommutators $\{c_i, c_j\}$ are all zero for any i, j. However, the creation and destruction operators have the more interesting relations $[a_i, a_j^\dagger] = \delta_{ij}$ and $\{c_i, c_j^\dagger\} = \delta_{ij}$. These operator relations carry the information about antisymmetrization of many-Fermion states and symmetrization of many-Boson states; putting these properties onto operators in a somewhat abstract Fock space turns out to be much simpler than keeping track of these properties for many particle wavefunctions in a more conventional Hilbert space. For related reasons, it turns out that superconductivity is very hard to describe in a conventional Hilbert space where the number of electrons is fixed, but becomes fairly easy in a Fock space where any number of electrons is allowed.

Here are some other useful relations. I write down only the Fermion versions. The Boson versions can be easily guessed. We introduce "field operators" $\hat{\psi}^\dagger(x) = \hat{\psi}_\sigma^\dagger(\vec{r})$ and $\hat{\psi}(x') = \hat{\psi}_{\sigma'}(\vec{r}')$, which create electrons at $x = (\vec{r}, \sigma)$, and destroy electrons at $x' = (\vec{r}', \sigma')$.

$$\hat{\psi}(x) = \hat{\psi}_\sigma(\vec{r}) = \sum_i \psi_i(x) c_i = \sum_{k,\sigma} \psi_{k\sigma}(\vec{r}) c_{k\sigma}. \tag{3}$$

Note that the convenient composite indices $x = (\vec{r}, \sigma)$ and $i = (k, \sigma)$ and $k = (\vec{k}, n)$ are used. The wavefunction $\psi_{k\sigma}(\vec{r})$ is most often independent of the spin direction σ, except in magnetic materials or for cases where the spin-orbit effect is important. The field operators obey the anticommutation relations

$$\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} = \{\hat{\psi}_\sigma(\vec{r}), \hat{\psi}_{\sigma'}^\dagger(\vec{r}')\} = \delta(\vec{r} - \vec{r}')\delta(\sigma, \sigma') = \delta(x, x'). \tag{4}$$

A single-particle operator like momentum (p_x) appears in many-particle physics as a collective operator $\hat{p}_x = \sum_\nu p_{\nu x}$ where ν enumerates all the identical particles whose momentum is under discussion. The single-particle collective operator $\hat{T}$ has an alternate representation in creation and destruction operators,

$$\begin{aligned} \hat{T} &= \int dx dx' \hat{\psi}^\dagger(x) T(x, x') \hat{\psi}(x') = \sum_{i,j} < i|T|j > c_i^\dagger c_j \\ &= \sum_{\sigma,\sigma'} \int d\vec{r} d\vec{r}' \hat{\psi}_\sigma^\dagger(\vec{r}) T_{\sigma,\sigma'}(\vec{r}, \vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') = \sum_{k\sigma, k'\sigma'} < k\sigma|T|k'\sigma' > c_{k\sigma}^\dagger c_{k'\sigma'}. \end{aligned} \tag{5}$$

This is written for the most general case. Almost always the single-particle operator $\hat{T}$ is local in space, meaning that $T_{\sigma,\sigma'}(\vec{r}, \vec{r}')$ simplifies to $T_{\sigma,\sigma'}(\vec{r})\delta(\vec{r} - \vec{r}')$. Also, except for operators which probe magnetic properties, the operator $\hat{T}$ is diagonal in spin, that is $T_{\sigma,\sigma'} = T\delta(\sigma, \sigma')$. As an example, the density operator $\hat{\rho}(\vec{r})$ in the $\vec{r}$-representation of ordinary Hilbert space is $\sum_\nu \delta(\vec{r} - \vec{r}_\nu)$. This is local in space and sums over all electrons independent of spin, so it is spin-diagonal. Applying equation 5, this becomes either

$$\hat{\rho}(\vec{r}) = \sum_\sigma \hat{\psi}_\sigma^\dagger(\vec{r}) \hat{\psi}_\sigma(\vec{r})$$

or

$$\hat{\rho}(\vec{r}) = \sum_{k,k',\sigma} \psi_{k\sigma}^*(\vec{r}) \psi_{k'\sigma}(\vec{r}) c_{k\sigma}^\dagger c_{k'\sigma}.$$

The operator $c_i^\dagger c_i$ is the number operator $\hat{n}_i$ whose expectation value is the number of electrons in state i (recall the analogous formula for phonons.) For a non-interacting system of Fermions whose eigenstates are $\psi_i(\vec{r})$ and eigenenergies ϵ_i, the expectation value $< c_i^\dagger c_i >$ of the number operator is (if the system is in thermal equilibrium) the Fermi-Dirac distribution $f_i = (\exp(\beta(\epsilon_i - \mu) + 1)^{-1}$.

There is a similar prescription for two particle operators such as pairwise interactions. If in the usual Hilbert space we have a spin-independent interaction $\hat{V} = {}^1\!/_2 \sum_{\mu,\nu} v(\vec{r}_\mu - \vec{r}_\nu)$, then this operator in Fock space is

$$\begin{aligned} \hat{V} &= \frac{1}{2} \int d\vec{r} d\vec{r}' \hat{\rho}(\vec{r}) v(\vec{r} - \vec{r}') \hat{\rho}(\vec{r}') \\ &= \frac{1}{2} \sum_{abcd} < ab|v|cd > c_{a\sigma}^\dagger c_{b\sigma} c_{c\sigma'}^\dagger c_{d\sigma'}. \end{aligned} \tag{6}$$