Lecture 16: Many-body physics in second-quantized language

In the last lecture, we went over two sets of algebraic preliminaries: One having to do with the abstract algebra of creation and annihilation operators for fermions and bosons, with defining relations consisting of anticommutators in the case of fermions and commutators in the case of bosons, and the other having to do with the nature of the many-boson and many-fermion Hilbert spaces, which consist of states which are totally symmetric under particle interchange for bosons and totally antisymmetric under particle interchange for fermions. That the latter is true is a fact of nature as far as anybody has been able to tell, and thus a basic physical input one must provide for the ensuing discussion.

Now, we define operations that add or remove particles from one of these many-particle states. The algebraic properties of these operations will be seen to follow the abstract operator algebra defined in the previous lecture, allowing one to represent the physics of many-body systems using the language provided by these operators.

First, we define an operation $a^\dagger(\phi)$ that adds a particle in a single-particle state $|\phi\rangle$ to the many-body state $|\psi_1 \cdots \psi_n\rangle_\zeta$ that originally has n indistinguishable particles (fermions if $\zeta = -1$, bosons if $\zeta = +1$)

$$a^\dagger(\phi)|\psi_1, \cdots, \psi_n\rangle_\zeta = |\phi, \psi_1 \cdots \psi_n\rangle_\zeta \tag{1}$$

For consistency, we also postulate that the single particle state $|\phi\rangle$ itself can be obtained from the vacuum state $|0\rangle_\zeta$ by the action of this creation operator:

$$|\phi\rangle = a^\dagger(\phi)|0\rangle_\zeta \tag{2}$$

We now ask: What is the adjoint of this operation? To answer this, denote the adjoint as usual by $a(\phi)$ and note that

$$\begin{aligned} {}_\zeta\langle x_1 \cdots x_{n-1}|a(\phi)|\psi_1 \cdots \psi_n\rangle_\zeta &= \left({}_\zeta\langle \psi_1 \cdots \psi_n|a^\dagger(\phi)|x_1 \cdots x_{n-1}\rangle_\zeta \right)^\star \\ &= {}_\zeta\langle \psi_1 \cdots \psi_n|\phi, x_1 \cdots x_{n-1}\rangle_\zeta^\star \end{aligned} \tag{3}$$

From the previous lecture, we know that this can be written as

$${}_\zeta\langle \psi_1 \cdots \psi_n|\phi, x_1 \cdots x_{n-1}\rangle_\zeta^\star = \begin{vmatrix} \langle\psi_1|\phi\rangle & \langle\psi_1|x_1\rangle & \cdots & \langle\psi_1|x_{n-1}\rangle \\ \vdots & \vdots & & \\ \langle\psi_n|\phi\rangle & \langle\psi_n|x_1\rangle & \cdots & \langle\psi_n|x_{n-1}\rangle \end{vmatrix}_\zeta^\star \tag{4}$$

For $\zeta = -1$ (fermions) we may expand this in terms of minors along the first column to get

$$\begin{vmatrix} \langle\psi_1|\phi\rangle & \langle\psi_1|x_1\rangle & \cdots & \langle\psi_1|x_{n-1}\rangle \\ \vdots & \vdots & & \\ \langle\psi_n|\phi\rangle & \langle\psi_n|x_1\rangle & \cdots & \langle\psi_n|x_{n-1}\rangle \end{vmatrix}_\zeta^\star = \sum_{k=1}^{n} \zeta^{k-1}\langle\phi|\psi_k\rangle\langle x_1\cdots x_{n-1}|\psi_1\cdots(\text{no }\psi_k)\cdots\psi_n\rangle \tag{5}$$

Moreover, by working directly with the definition of the many-boson state given in the previous lecture, it is easy to see that the same final expression also holds for bosons, so we may use the same final expression for either sign of ζ. Since this is true for arbitrary $|x_1\cdots x_{n-1}\rangle$, we can write

$$a(\phi)|\psi_1\cdots\psi_n\rangle = \sum_{k=1}^{n} \zeta^{k-1}\langle\phi|\psi_k\rangle|\psi_1\cdots(\text{no }\psi_k)\cdots\psi_n\rangle \tag{6}$$

So $a(\phi)$ removes one particle from among those occupying the single particle state $|\phi\rangle$ and attaches a sign (for fermions) that depends on the convention used for ordering single-particle states.

From this it is now clear that

$$[a(\phi_1), a(\phi_2)]_\zeta = 0. \tag{7}$$

where $[A, B]_{\zeta=+1} = AB - BA$, while $[A, B]_{\zeta=-1} = AB + BA$.

Moreover, from the original definiton

$$a^\dagger(\phi)|\psi_1\cdots\psi_n\rangle = |\phi, \psi_1\cdots\psi_n\rangle\ , \tag{8}$$

it is also clear that

$$[a^\dagger(\phi_1), a^\dagger(\phi_2)]_\zeta = 0 \tag{9}$$

These commutation/anticommutation properties are identical to those of the algebra of creation and annihilation operators we studied in the previous lecture (in the previous lecture, we studied only one pair of operators a and $a^\dagger$, but the discussion in that lecture clearly generalizes to many independent pairs, where by independent we mean things that commute in the case of bosons and anticommute in the fermionic case). Indeed, that was the reason for choosing to study it. To complete the connection, we need to work out

$[a(\phi_1), a^\dagger(\phi_2)]_\zeta$. To do this, note that

$$\begin{aligned} a(\phi_1)a^\dagger(\phi_2)|\psi_i \cdots \psi_n\rangle &= a(\phi_1)|\phi_2\psi_1 \cdots \psi_n\rangle \\ &= \sum_{k=1}^{n} \zeta^k \langle\phi_1|\psi_k\rangle|\phi_2, \psi_1 \cdots \text{no } \psi_k \cdots \psi_n\rangle + \langle\phi_1|\phi_2\rangle|\psi_1 \cdots \psi_n\rangle \end{aligned} \tag{10}$$

Likewise

$$\begin{aligned} a^\dagger(\phi_2)a(\phi_1)|\psi_1 \cdots \psi_n\rangle &= a^\dagger(\phi_2) \sum_{k=1}^{n} \zeta^{k-1} \langle\phi_1|\psi_k\rangle|\psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n\rangle \\ &= \sum_{k=1}^{n} \zeta^{k-1} \langle\phi_1|\psi_k\rangle|\phi_2, \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n\rangle \\ &= \zeta \sum_{k=1}^{n} \zeta^{k} \langle\phi_1|\psi_k\rangle|\phi_2, \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n\rangle \end{aligned} \tag{11}$$

So we have

$$(a(\phi_1)a^\dagger(\phi_2) - \zeta a^\dagger(\phi_2)a(\phi_1))|\psi_1 \cdots \psi_n\rangle = \langle\phi_1|\phi_2\rangle|\psi_1 \cdots \psi_n\rangle \tag{12}$$

Since this holds for an arbitrary state, we have the operator equation

$$[a(\phi_1), a^\dagger(\phi_2)]_\zeta = \delta_{\phi_1,\phi_2} \tag{13}$$

since we are using orthonormal single particle states with $\langle\phi_1|\phi_2\rangle = \delta_{\phi_1,\phi_2}$.

At this point, it is important to recognize that the many-particle states $|\psi_1 \cdots \psi_n\rangle_\zeta$ used in the above are un-normalized in the Bose case since more than one particle can occupy the same single particle state (as discussed in the previous lecture).

From now on, we normalize these states to unit norm as in the previous lecture, and denote the corresponding normalized n-particle states by the notation $|n_1, n_2, \cdots\rangle_\zeta$, where $n_1 + n_2 \cdots = n$ is the total number of particles, and the integers n_k tell us how many times a given single particle state ψ_k appears in $|\psi_1 \cdots \psi_n\rangle_\zeta$, *i.e.* how many particles occupy this single particle state. In terms of these normalized states, it is easy to use the foregoing to conclude that

$$\begin{aligned} a_\alpha^\dagger|n_1, n_2, \cdots, n_\alpha, \cdots\rangle &= \sqrt{n_\alpha + 1}|n_1, n_2, \cdots, n_\alpha + 1, \cdots\rangle \\ a_\alpha|n_1, n_2, \cdots, n_\alpha, \cdots\rangle &= \sqrt{n_\alpha}|n_1, n_2, \cdots, n_\alpha - 1, \cdots\rangle \end{aligned} \tag{14}$$

From this, and the commutation/anticommutation relations obtained above, it is clear that the integers n_α are in fact eigenvalues of the "number operator"

$$n_\alpha = a_\alpha^\dagger a_\alpha \tag{15}$$

defined in the previous lecture in our study of the abstract algebra of creation and annihilation operators. Thus, this operator is really the number of particles in single-particle state ψ_α, and we simply need to use many copies of this abstract algebra (one for each α) to have a complete language for describing the quantum mechanics of many-particle systems. In this context, it is again important to note that these copies are "independent" of each other, where independence means that things commute for different α in the bosonic case, and things *anticommute* for different α in the fermionic case.

In using this formalism, one typically uses a complete set of position or momentum eigenstates as the single-particle basis. In other words, one typically works either with operators a_x and $a_x^\dagger$ satisfying

$$[a_x, a_{x'}^\dagger]_\zeta = \delta^d(x - x') \tag{16}$$

(d is the spatial dimension) and all other commutators (anticommutators) equal to zero for bosons (fermions), or with operators a_p and $a_p^\dagger$ satisfying

$$[a_p, a_{p'}^\dagger]_\xi = \langle p|p'\rangle = (2\pi)^d \delta^d(p - p') \tag{17}$$

with all other commutators (anticommutators) equal to zero for bosons (fermions).

Therefore, one question that arises immediately is: What is the relation between these two sets of operators? To answer this, it is useful to first define creation operators that create a particle in a linear superposition of two single-particle states: If

$$|\chi\rangle = \alpha|\psi\rangle + \beta|\phi\rangle \tag{18}$$

then we define

$$a_\chi^\dagger \equiv \alpha a_\psi^\dagger + \beta a_\phi^\dagger \tag{19}$$

This immediately implies that

$$a_\chi = \alpha^\star a_\psi + \beta^\star a_\phi \tag{20}$$

With this in hand, we may use the fact that

$$|p\rangle = \int d^d x e^{ipx} |x\rangle \tag{21}$$

to write

$$\begin{aligned} a_p^\dagger &= \int d^d x e^{ipx} a_x^\dagger \\ a_x^\dagger &= \int \frac{d^d p}{(2\pi)^d} e^{-ipx} a_p^\dagger \end{aligned} \tag{22}$$

In other words, these two sets of operators are operator-valued Fourier transforms of each other.

With this background, let us ask how we may represent typical terms in the Hamiltonian of a system of interacting particles. Typically, particles are subjected to a external potential, which we term a "one-body operator" in this context for obvious reasons. In addition, they feel the effects of other particles due to the presence of inter-particle interactions between any pair of particles. For obvious reasons, such interactions are classified as "two-body operators". In addition, one can have three-body interactions present in certain effective models of strongy-correlated electronic systems, although the basic non-relativistic Coulomb interaction between electrons is a pair-wise interaction, and therefore a two-body term in the Hamiltonian.

How do we represent a one-body operator in this formalism? To answer this, we write a general one body operator as

$$A = \sum_{i=1} A(i) \tag{23}$$

where the argument i reminds us that the i^{th} term acts only on the Hilbert space of the i^{th} particle. An example is an external potential V that all particles feel

$$V = \sum_i V(x_i) \tag{24}$$

In this case, the operator acting in the Hilbert space of the i^{th} particle is written in the position basis, and x_i is the d-dimensional coordinate of the i^{th} particle.

Next, we suppose for the time being that each $A(i)$ has a very simple form $|\alpha\rangle\langle\beta|$ where $|\alpha\rangle$ and $|\beta\rangle$ are orthonormal basis states in the Hilbert space of the i^{th} particle. Then

$$A|\psi\rangle_\zeta = \langle\beta|\psi_1\rangle|\alpha, \psi_2 \cdots \psi_n\rangle_\zeta + \langle\beta|\psi_2\rangle|\psi_1, \alpha, \cdots \psi_n\rangle_\zeta + \cdots \langle\beta|\psi_n\rangle|\psi_1 \cdots \psi_{n-1}\alpha\rangle_\zeta \tag{25}$$

Now, we compare this with the action of $a^\dagger_\alpha a_\beta$:

$$\begin{aligned} a^\dagger_\alpha a_\beta|\psi\rangle_\zeta &= \sum_{k=1}^{n} \xi^{k-1}\langle\beta|\psi_k\rangle|\alpha, \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n\rangle_\zeta \\ &= \sum_{k=1}^{n} \langle\beta|\psi_k\rangle|\psi_1 \cdots (\alpha \text{ instead of } \psi_k) \cdots \psi_n\rangle_\zeta \end{aligned} \tag{26}$$

Comparing the two, we see that in this special case

$$A = a^\dagger_\alpha a_\beta \ . \tag{27}$$

Since any A can be written as a sum of terms of this form, with coefficients $A_{\alpha\beta}$ that are up to us to specify, we may write

$$A = \sum_{\alpha\beta} A_{\alpha\beta} a^\dagger_\alpha a_\beta \tag{28}$$

for a general single particle operator.

To fix this in our minds, let us consider again the case of the external potential $V(x)$. Since this is diagonal in the x basis, we have the expression

$$V = \int d^d x V(x) a^\dagger_x a_x. \tag{29}$$

Another useful-to-note example is a one-body operator

$$N = \sum_i \mathbf{1}_i \tag{30}$$

where $\mathbf{1}_i$ is the identity in the Hilbert space of the i^{th} particle. This just measures the total number of particles, and clearly has the representation

$$N = \int d^d x a^\dagger_x a_x \tag{31}$$

Similarly, the total momentum operator is most conveniently represented as

$$P_\mu = \int \frac{d^d p}{(2\pi)^d} p_\mu a_p^\dagger a_p \tag{32}$$

With this in hand, let us now turn to two-body operators, focusing on the example of a pair-wise interaction U. Clearly, it is convenient to work in the position basis. In this basis, we want a operator U that acts on the n particle state in the following way

$$\begin{aligned} U|x_1 \cdots x_n\rangle_\zeta &= \sum_{i<j} U(x_i, x_j)|x_1 \cdots x_n\rangle_\zeta \\ &= \frac{1}{2}\sum_{i,j} U(x_i, x_j)|x_1 \cdots x_n\rangle_\zeta \end{aligned} \tag{33}$$

How do we mimic this action using an expression made up of creation and annihilation operators? The obvious (by now) guess is an expression of the type

$$\frac{1}{2}\int a_x^\dagger a_y^\dagger a_y a_x U(x,y) d^d x d^d y. \tag{34}$$

I leave it to you to work through the simple algebra involved and check that this is indeed true. This concludes our discussion of many-body formalism.

With this formalism, the effective Hamiltonian for the tight-banding one-band representation of the Cu-O plane of cuprate superconductors can now be written compactly as

$$H = -t\sum_{\langle ij\rangle}(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U\sum_i n_{i\uparrow} n_{i\downarrow} \tag{35}$$

where $\langle ij\rangle$ denote links connecting nearest neighbour points i and j of the square lattice, $\sigma = \uparrow, \downarrow$ are the two spin polarizations of the electron along some quantization axis, and $c_{i\sigma}$ annihilates an electron at site i with spin polarization σ.

Using this language, it is possible to now repeat the perturbative derivation of the Heisenberg antiferromagnet Hamiltonian in the $U \gg t$ limit at half-filling without introducing any "fermionic" minus signs by hand every time particles are interchanged. Similarly, it is possible to study bosonic versions of the above, of possible relevance to the physics of ultra-cold bosonic atoms with two degenerate hyperfine states in an atom-trap experiment. I leave both to you as self-assessment exercises, detailed separately.