Lecture 15: Many-particle quantum mechanics: Algebraic preliminaries and wavefunction description

In the last module, we have seen how a simple perturbative calculation of the effective Hamiltonian for the one-band Hubbard model in the limit of large U/t at half-filling already presents difficulties for our standard single-particle quantum mechanics formalism because of the many-body nature of the system, in which the number of particles can vary, and where the many-particle states acquire statistical phases when fermionic particles are exchanged. Indeed, if you recall our derivation of the Heisenberg exchange Hamiltonian in this limit, keeping track of these minus signs "by hand" in the exchange term was crucial—without this, it was not possible to obtain the correct rotationally invariant (in spin-space) effective Hamiltonian.

Although the basic framework of quantum mechanics remains essentially unchanged and is perfectly capable of handling such many particle systems, we need a better language to keep track of such statistical phase factors and the variations in particle number. This is the formalism of "second-quantization" (the terminology is largely a legacy of history, and there is no real sense in which there is an additional quantization being postulated or performed). In this lecture, we will introduce this convenient formalism, and then revisit our derivation of Heisenberg exchange Hamiltonian to see how the new language allows us to "automate" considerations related to the statistical phase picked up by the wavefunction under interchange of particles.

With this motivation in mind, let us begin with a mathematical preliminary: Suppose we had two operator a, $a^\dagger$ (where $a^\dagger$ is of course the hermitean conjugate of a) satisfying

$$[a, a^\dagger] = 1 \ . \tag{1}$$

What can we say about about the eigenvalues of the Hermitean operator

$$a^\dagger a \equiv \hat{n} \ ? \tag{2}$$

The first statement we can of course make is that the eigenvalues are real since the operator is Hermitean.

A little thought also convinces us that the eigenvalues must be positive (but not necessarily positive definite). For if

$$\hat{n}|\phi\rangle = \phi|\phi\rangle \ , \tag{3}$$

where $|\Phi\rangle$ is a normalized eigenvector. Then

$$\begin{aligned} \phi &= \langle\phi|\hat{n}|\phi\rangle \\ &= \|a|\phi\rangle\|^2 \\ &\geq 0 \, . \end{aligned} \tag{4}$$

Thus eigenvalues of $\hat{n}$ are real and positive. What else can we say? Well, another easy-to-see property is that

$$a|\phi\rangle \propto |\phi - 1\rangle \, . \tag{5}$$

To see this, we note that

$$\hat{n}a|\phi\rangle = \phi a|\phi\rangle + [\hat{n}, \hat{a}]|\phi\rangle \, , \tag{6}$$

and observe that

$$\begin{aligned} [a^\dagger a, a] &= a^\dagger [a, a] + [a^\dagger, a]a \\ &= -a \, . \end{aligned} \tag{7}$$

Therefore, we have

$$\hat{n}a|\phi\rangle = (\phi - 1)a|\phi\rangle \, . \tag{8}$$

In a completely analogous manner, we see that

$$a^\dagger|\phi\rangle \propto |\phi + 1\rangle \, . \tag{9}$$

Thus, if ϕ is an eigenvalue, so are $\phi \pm 1$, $\phi \pm 2 \cdots$ so long as the state in question does not have zero norm. Therefore, if ϕ is an eigenvalue, so is $\phi - m$ for every positive integer m such that $\|(a)^m|\phi\rangle\| > 0$. Now, since all eigenvalues of $\hat{n}$ are positive, it must therefore be true that $\|(a)^m|\phi\rangle\| = 0$ for m such that $\phi - m$ is negative.

Let $|\Psi\rangle$ be the normalized eigenvector corresponding to the smallest eigenvalue Ψ. If Ψ is the smallest eigenvalue, it must be true that $\|a|\Psi\rangle\| = 0$. But $\|a|\Psi\rangle\|^2 = \Psi$. Therefore,

$$\Psi = 0 \, . \tag{10}$$

Thus, eigenvalues of $\hat{n}$ are $0, 1, 2, 3 \ldots \infty$. If we denote the normalized eigenstate with eigenvalue 0 by $|0\rangle$, and that with eigenvalue m as $|m\rangle$. Then we have

$$|m\rangle \propto a^\dagger|m - 1\rangle \, . \tag{11}$$

To fix the normalization, we note that

$$\begin{aligned} \|a^\dagger|m-1\rangle\|^2 &= \langle m-1|aa^\dagger|m-1\rangle \\ &= \langle m-1|a^\dagger a+1|m-1\rangle \\ &= m \end{aligned} \tag{12}$$

Therefore, we have

$$|m\rangle = \frac{1}{\sqrt{m}}a^\dagger|m-1\rangle \; . \tag{13}$$

This allows us to write

$$|m\rangle = \frac{1}{\sqrt{m!}}|0\rangle \; . \tag{14}$$

As a consequence, we have the basic relations

$$\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\ a|n\rangle &= \sqrt{n}|n-1\rangle \; . \end{aligned} \tag{15}$$

With an eye to using this formalism to describe multi-particle states of bosons with variable numbers of particles in various single-particle eigenstates, we refer to a as the particle-annihilation operator, $a^\dagger$ as the creation operator and $\hat{n}$ as the number operator.

What about Fermions? Well, it turns out that the simplest way to capture the fact that Fermions obey the Pauli exclusion principle to work with creation and annihilation operators that satisfy a different algebra, in which their anticommutator plays a key role:

$$\begin{aligned} \{a, a^\dagger\} &= 1 \\ \{a, a\} &= 0 \\ \{a^\dagger, a^\dagger\} &= 0 \end{aligned} \tag{16}$$

What can we now say about the corresponding fermionic number operator $a^\dagger a = \hat{n}$? Well, we proceed again in a similar way: If $|\phi\rangle$ is a normalized eigenvector, we note that

$$\|a|\phi\rangle\|^2 = \phi \; . \tag{17}$$

Therefore, $\|a|\phi\rangle\| = 0$ if and only if $\phi = 0$. But

$$\begin{aligned} \hat{n}a|\phi\rangle &= a^\dagger a^2|\phi\rangle \\ &= 0 \; . \end{aligned} \tag{18}$$

. Therefore, we must either have $\|a|\phi\rangle\| = 0$ and $\phi = 0$ or $a|\phi\rangle \propto |0\rangle$. Therefore, one eigenvalue is $\phi = 0$, and we denote the corresponding normalized eigenvector by $|0\rangle$.

Next, we note that

$$\begin{aligned} \|a^\dagger|\phi\rangle\|^2 &= \langle\phi|aa^\dagger|\phi\rangle \\ &= \langle\phi|\phi\rangle - \langle\phi|a^\dagger a|\phi\rangle \\ &= (1-\phi)\,. \end{aligned} \tag{19}$$

Therefore, we must have $\phi \leq 1$. Finally, we note that

$$\begin{aligned} \hat{n}a^\dagger|0\rangle &= a^\dagger aa^\dagger|0\rangle \\ &= a^\dagger(1-a^\dagger a)|0\rangle \\ &= a^\dagger|0\rangle \end{aligned} \tag{20}$$

Therefore, another eigenvalue is $\phi = 1$, and the corresponding normalized eigenvector, which may label by $|1\rangle$, is proportional to $a^\dagger|0\rangle$. Since any eigenvalue with $\phi \neq 0$ must satisfy $a|\phi\rangle \propto |0\rangle$, and since

$$\begin{aligned} aa^\dagger|0\rangle &= (1-a^\dagger a)|0\rangle \\ &= |0\rangle\,, \end{aligned} \tag{21}$$

we conclude that the only other eigenvector is $|1\rangle$. Indeed, we have

$$\begin{aligned} a|1\rangle &= |0\rangle\,, \\ a^\dagger|0\rangle &= |1\rangle\,, \\ a|0\rangle &= 0\,, \\ a^\dagger|1\rangle &= 0\,. \end{aligned} \tag{22}$$

Thus, this algebra captures the fact that Pauli exclusion limits the occupation of any single-particle level to exclude two identical fermions ever occupying the same level.

After this algebraic prelude, let us turn to the description of systems with many identical particles, either bosonic or fermionic in nature. If we had n distinguishable particles and the 1st particle was in quantum state $|\psi_1\rangle$, second in state $|\psi_2\rangle$ and so on$\cdots$, we would write

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots |\psi_n\rangle \tag{23}$$

where the tensor product notation reminds us that the first slot corresponds to the Hilbert space of the first particle, the second to that of the second particle and so on. But if particles are indistinguishable, no observable should be affected if we make the "1st" particle and "kth" particle switch roles. $|\psi\rangle$ written above does not have this property. One obvious way of guaranteeing this is to consider the symmetrized version of the above

$$|\psi\rangle_s = \frac{1}{\sqrt{n!}} \sum_{\mathcal{P}} |\psi_{\mathcal{P}(1)}\rangle \otimes |\psi_{\mathcal{P}(2)}\rangle \otimes \cdots |\psi_{p(n)}\rangle \tag{24}$$

where $\mathcal{P}$ is a permutation of the labels $1, 2, 3 \ldots$. Now, we can no longer say a definite particle has a definite quantum state, just that we have n particles that occupy states $(\psi_1 \cdots \psi_n)$.

It seems to be a fact of nature that the only allowed states of systems made up of many identical bosonic particles are constructed from various linear combinations of different $|\psi\rangle_s$. For systems made up of many identical fermionic particles, indistinguishable particles, the states that describe physical reality seem to also take into account their fundamental indistinguishability, but in a different way. This difference is linked to the fact that fermions obey the Pauli exclusion principle, and leads to the presence of minus signs that keep track of whether a given term corresponds to an odd permutation:

$$|\psi\rangle_a = \frac{1}{\sqrt{n!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} |\psi_{\mathcal{P}(1)}\rangle |\psi_{\mathcal{P}(2)}\rangle \cdots \psi_{\mathcal{P}(n)}\rangle \tag{25}$$

It appears to be a basic fact of nature that the only allowed states of many-fermion systems are linear combinations made up of various $|\psi\rangle_a$.

It is instructive to restate this in coordinate-space wavefunction language: For distinguishable particles, we would have constructed many-particle basis states in which the i$^{\text{th}}$ particle is at position x_i:

$$|x_1\rangle |x_2\rangle \cdots |x_n\rangle \tag{26}$$

However, for indistinguishable bosons, we now see that we must instead use the symmetrized version

$$|x\rangle_s = \frac{1}{\sqrt{n!}} \sum_{\mathcal{P}} |x_{\mathcal{P}(1)}\rangle |x_{\mathcal{P}(2)}\rangle \cdots |x_{\mathcal{P}(n)}\rangle \tag{27}$$

while for fermions we must use

$$|x\rangle_s = \frac{1}{\sqrt{n!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} |x_{\mathcal{P}(1)}\rangle |x_{\mathcal{P}(2)}\rangle \cdots |x_{\mathcal{P}(n)}\rangle \tag{28}$$

Any correctly symmetrized bosonic state $|\psi\rangle_s$ or antisymmetrized fermionic state $|\psi\rangle_a$ can be expanded in terms of these basis states. The coefficients $\langle x|\psi\rangle_s$ and $\langle x|\psi\rangle_a$ have compact expressions in terms of *permanents* and *determinants* of the matrix

$$\langle x|\psi\rangle_\zeta = \left| \begin{array}{c} \langle x_1|\psi_1\rangle \cdots \langle x_1|\psi_n\rangle \\ \vdots \\ \langle x_n|\psi_1\rangle \cdots \langle x_n|\psi_n\rangle \end{array} \right|_\zeta \qquad \begin{array}{rcl} \zeta & = & +1 \text{ ors} \\ & & \\ & = & -1 \text{ ora} \end{array}$$

where

$$|A|_\zeta = \sum_{\mathcal{P}} \zeta^{\mathcal{P}} A_{1\mathcal{P}(1)} A_{2\mathcal{P}(2)} \cdots A_{n\mathcal{P}(n)}. \tag{29}$$

Here, the expression with $\zeta = -1$ is the standard determinant of A, while that with $\zeta = +1$ is called the *permanent*.

The proof of this claim is straightforward. We note that

$$\langle x|\psi\rangle \;=\; \frac{1}{n!} \sum_{P,Q} \zeta^P \zeta^Q \langle x_{P(1)}|\psi_{Q(1)}\rangle \langle x_{P(2)}|\psi_{Q(2)}\rangle \cdots \tag{30}$$

Changing variables in the first sum over P, we may rewrite this as

$$\begin{aligned} \langle x|\psi\rangle &= \frac{1}{n!} \sum_P \sum_Q \zeta^P \zeta^Q \langle x_1|\psi_{QP^{-1}(1)}\rangle \langle x_2|\psi_{QP^{-1}(2)}\rangle \cdots \\ &= \frac{1}{n!} \sum_P \sum_Q \zeta^{QP^{-1}} \langle \cdots\rangle\langle \cdots\rangle \cdots \\ &= \frac{1}{n!} \sum_P \sum_R \zeta^R \langle x_1|\psi_{R(1)}\rangle \cdots \\ &= |\langle x|\psi\rangle|_\zeta \,, \end{aligned} \tag{31}$$

as claimed above.

Now, if the $\{|\alpha\rangle\}$ form a complete set of orthonormal single particle states, then all n particle bosonic states can be written in terms of $|\alpha_1, \alpha_2, \cdots, \alpha_n\rangle_\zeta$ where we take some subset of the α: $\alpha_1 \leq \alpha_2 \leq \alpha_3 \cdots \leq \alpha_n$. If we are to construct n particle fermion states, we must take a set of α without any repetitions: $\alpha_1 < \alpha_2 < \alpha_3 \cdots \alpha_n$, so as to satisfy the Pauli exclusion principle.

In the fermionic case, the state $|\alpha_1, \alpha_2, \cdots, \alpha_n\rangle_{\zeta=-1}$ is already normalized. However, in the bosonic case, it is not normalized. To figure out the normalization, we begin by writing

$$ {}_+\langle \alpha_1 \cdots \alpha_n | \alpha_1 \cdots \alpha_n \rangle_+ = \sum_P \langle \alpha_1 | \alpha_{P(1)} \rangle \cdots \langle \alpha_n | \alpha_{P(n)} \rangle. \tag{32} $$

where the sum over permultations on the left has been cancelled off against the overall denominator of $n!$ coming from the normalization used for the bra and the ket. Now, let the sequence $\alpha_1 \cdots \alpha_n$ be made of n_1 repetitions of α_1, n_2 repetitions of α_2 and so on $\cdots$, with the final entries being n_k repetitions of α_k. Then there are $(n_1!)(n_2!)(n_3!)\cdots(n_k!)$ permutations that contribute to this overlap. So, to normalize the bosonic state, we must introduce a corresponding prefactor and write

$$ |\overline{\alpha_1 \cdots \alpha_n}\rangle_\zeta = \frac{1}{\sqrt{n_1! n_2! \cdots}} |\alpha_1 \cdots \alpha_n\rangle_\zeta \ . \tag{33} $$

In terms of the $|\alpha_1 \cdots \alpha_n\rangle_\zeta$, we have the obvious completeness relation in the n-particle sector of the many-particle Hilbert space

$$ \sum_{\{\alpha_1 \cdots \alpha_n\}} |\overline{\alpha_1 \cdots \alpha_n}\rangle_\zeta \ {}_\zeta\langle \overline{\alpha_1 \cdots \alpha_n}| = \mathbb{1}_\zeta \tag{34} $$

where the sum is over single-particle quantum numbers satisfying $\alpha_1 \leq \alpha_2 \leq \cdots \alpha_n$ for bosons and $\alpha_1 < \alpha_2 \cdots \alpha_n$ for fermions. To describe a varying number of particles, we may simply superpose states from sectors with different number of particles thus:

$$ |\psi\rangle_\zeta = |\psi^{(0)}\rangle_\zeta + |\psi^{(1)}\rangle_\zeta \cdots |\psi^n\rangle_\zeta \tag{35} $$

where $|\psi^0\rangle_\zeta \equiv |0\rangle$ is the *vacuum state* with no particles. is appropriate n particle state. Clearly, we require any $\langle \psi^{(m)} | \psi^{(n)} \rangle_\zeta = 0$ for $m \neq n$. So we have

$$ \langle \phi | \psi \rangle_\zeta = \delta_{nm} \begin{vmatrix} \delta_{\alpha_1\beta_1} \cdots \delta_{\alpha_1\beta_n} \\ \delta_{\alpha_n\beta_1} \cdots \delta_{\alpha_n\beta_n} \end{vmatrix}_\zeta \tag{36} $$

for many-particle states constructed from orthonormal single particle states.

Finally, for any fixed n, the completeness relation can also be rewritten as

$$\frac{1}{n!}\sum_{\alpha_1,\alpha_2,\alpha_3,\alpha_n} |\alpha_1\cdots\alpha_n\rangle_\zeta\ {}_\zeta\langle\alpha_1\cdots\alpha_n| = \mathbb{1}_\zeta^{(n)} \tag{37}$$

where the sum over the single-particle quantum numbers is now an unrestricted sum. To see this, we simply note that going from $\sum_{\alpha_1\leq\alpha_2\cdots}$ to the unrestricted sum introduces an additional degeneracy of $n!/(n_1!n_2!\cdots)$. Allowing for superposition of states with different numbers of particles, the general completeness relation can thus be written as

$$\sum_n \frac{1}{n!}\sum_{\alpha_1,\alpha_2,\cdots,\alpha_n} |\alpha_1\cdots\alpha_n\rangle_\zeta\ {}_\zeta\langle\alpha_1\cdots\alpha_n| = \mathbb{1}_\zeta \tag{38}$$

Thus, we now understand how Bose and Fermi statistics are to be encoded in the properties of multi-particle states of a system of many indistinguishable particles, allowing for the possibility of quantum mechanical superposition of states with different number of particles. Although this language provides a complete and precise description of the relevant physics, it is not the most convenient one when it comes to calculations [the one exception is variational wavefunction studies, where one works directly with these multi-particle states and optimizes them to lower the energy so as to best approximate the ground state].

A much better description results from *constructing* these multi-particle states starting from the vacuum $|0\rangle$ using *creation* and *annihilation* operations whose algebra will turn out to be the same as the algebra of the a and $a^\dagger$ operators we have studied earlier in this lecture. This is what we will turn to in the next lecture.