Lecture notes FY8305

August, 2019

Contents

2

1 Short recap of second quantization for fermions and bosons

Pages 2-10 in lecture notes.

Notation: μ = set of quantum numbers that define a one-particle state.

1.1 Many particle basis

Ex 1.

$$\mu = (\vec{k}, \sigma) : \text{Wave number, spin}$$
$$\mu = (i, \sigma) : \text{Lattice point, spin}$$
$$\mu = (n, i) : \text{Orbital, lattice point}$$

A many-particle basis can be written $|\phi\rangle = |n_\mu, n_\nu, \ldots, n_{\mu_N}\rangle$. Many particle states are built by combining many one-particle states, but where the one-particle states are not necessarily independent. If <u>one</u> of the set of quantum numbers, μ_i, are changed, this <u>scattering</u> will generally have consequences for the distribution of quantum numbers for the remaining sets $\{\mu_j\}_{j \neq i}$. We generally imagine that many-particle states can be built as a linear combination of $|\phi\rangle$'s;

$$|\Psi\rangle = \sum_{n_{\mu_1}, \ldots, n_{\mu_N}} \phi_{\mu_1, \ldots, n_{\mu_N}} |\mu_1, \ldots, n_{\mu_N}\rangle. \tag{1}$$

A definite one-state vector $|n_\mu, \ldots, n_{\mu_N}\rangle$ can be demanded from a vacuum state (where there is no filled one-particle states) $|0\rangle$ via creation operators.

$$\textbf{bosons :} \qquad a_\mu^\dagger$$
$$\textbf{fermions :} \qquad c_\mu^\dagger$$

A quanta in a one-particle state can be destroyed by the annihilation operators.

$$\textbf{bosons :} \qquad a_\mu$$
$$\textbf{fermions :} \qquad c_\mu$$

These operators satisfy some commutation relations:

$$[a_\mu, a_\nu] = [a_\mu^\dagger, a_\nu^\dagger] = 0 \tag{2}$$
$$[a_\mu, a_\nu^\dagger] = \delta_{\mu\nu} \tag{3}$$
$$[A, B] = AB - BA \tag{4}$$
$$\{c_\mu^\dagger, c_\nu^\dagger\} = \{c_\mu, c_\nu\} = 0 \tag{5}$$
$$\{c_\mu, c_\nu^\dagger\} = \delta_{\mu\nu} \tag{6}$$
$$\{A, B\} = AB + BA \tag{7}$$

These will automatically satisfy the Pauli principle as well, which gives *symmetri/* antisymmetric solutions by exchange, dependent if the particles are bosons/fermions.

1.2 From classical formulation to second quantization of one-particle operators

For one-particle operators we usually have a kinetic energy function on a form like

$$T = \sum_i T\left(\vec{r}_i, \vec{p}_i\right) = \sum_i T\left(\vec{r}_i, \frac{\partial}{\partial r}\right) \tag{8}$$

Ex 2. External electrostatic potential:

$$T = \sum_i V_{\text{ext}}\left(\vec{r}_i\right) \tag{9}$$

Ex 3. Kinetic energy:

$$T = \sum_i \frac{p^2}{2m} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 \tag{10}$$

Ex 4. Crystal-potential:

$$T = \sum_i \sum_j v_{\text{cryst}}\left(\vec{r}_i, \vec{R}_j\right) \tag{11}$$

Second quantization by an operator on this form can be written

$$T = \sum_{\mu,\nu} T_{\mu\nu} c_\mu^\dagger c_\nu, \tag{12}$$

where

$$T_{\mu\,\nu} = \langle\mu|T\left(\vec{r},\vec{p}\right)|\nu\rangle. \tag{13}$$

Note: The matrix element of one-particle operators are determined by matrix elements in the Hilbert space of one-particle states.

1.3 From classical formulation to second quantization of two-particle operators

Typically, we consider pair-potentials

$$V = \sum_{i,j} V\left(\vec{r}_i, \vec{r}_j\right). \tag{14}$$

Ex 5. Exchange interaction of two charges

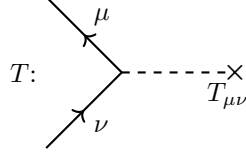$$V = \frac{e^2}{2} \sum_{i\neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \tag{15}$$

4

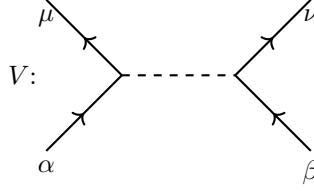Figure 1: Scattering from an external potential $v_{\mu\nu}c_\mu^\dagger c_\nu$

Figure 2: Exchange interaction between two particles.

The second quantization versions of these are

$$V = \sum_{\mu,\dots,\beta} V_{\mu\nu\alpha\beta}c_\mu^\dagger c_\nu^\dagger c_\alpha c_\beta, \tag{16}$$

where again

$$V_{\mu\nu\alpha\beta} = \langle\mu\nu|V\left(\vec{r}_i, \vec{r}_j\right)|\beta\alpha\rangle \tag{17}$$

Note: The matrix element of two-particle operators are determined by matrix elements in the Hilbert room of two-particle states.

The Hamiltonian:

$$H = T + V \tag{18}$$

$$T = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 \tag{19}$$

So far, we have just presented second quantization for fermion operators, but an equivalent statement will of course hold for the second quantization version of the Hamiltonian for an interacting, material, bosonic system, which has the same identical form as (18). Notice that each term in H has just as many $c_\mu^\dagger$ as c_ν.

1.4 Statistical mechanics

Assume that we know the spectrum E_N^n for an interacting many-particle system, defined by a state $|\psi_N\rangle_n$, where N is the number of particles in the system and n is an index that indicates what excited state $|\psi_N\rangle_n$ the system is in. $|\psi_N\rangle$ is also assumed to be known, such that the matrix product of observables can be calculated:

$$H\left|\psi\right\rangle_n = E_N\left|\psi\right\rangle_n. \tag{20}$$

To do statistical mechanics, we need to introduce temperature. We do this by using the canonical partition function

$$Z_N = \sum_n e^{-\beta E_N^n}. \tag{21}$$

Note, in (21) we sum over states, <u>not</u> the energy levels E_N^n.

$$\begin{aligned}
Z &= \sum_n {}_n \langle \psi_N | e^{-\beta H} | \psi_N \rangle_n \\
&= \text{Tr}\left(e^{-\beta H}\right) = \text{Tr}\left(S^{-1} S e^{-\beta H}\right) \\
&= \text{Tr}\left(S e^{-\beta H} S^{-1}\right) \\
&= \sum_{n'} {}_{n'} \langle \phi_N | e^{-\beta H} | \phi_N \rangle_{n'}.
\end{aligned} \tag{22}$$

We see in (22) that we can use an <u>arbitrary</u> basis to calculate the partition function. The most convenient basis is often a basis where the Hamiltonian is diagonal, but not always.

We write the statistical mean value of an operator as

$$\begin{aligned}
\left\langle \hat{O} \right\rangle &\equiv \frac{1}{Z} \text{Tr}\left(\hat{O} e^{-\beta H}\right) \\
&= \frac{1}{Z} \sum_n {}_n \langle \psi_N | \hat{O} e^{-\beta H} | \psi_N \rangle_n \\
&= \frac{1}{Z} \sum_{n,n'} {}_n \langle \psi_N | \hat{O} | \psi_N \rangle_{n'} \underbrace{{}_{n'} \langle \psi_N | e^{-\beta H} | \psi_N \rangle_n}_{\delta_{nn'} e^{-\beta E_{n'}}}.
\end{aligned} \tag{23}$$

Thus, we have

$$\left\langle \hat{O} \right\rangle = \frac{1}{Z} \sum_n \underbrace{{}_n \langle \psi_N | \hat{O} | \psi_N \rangle_n}_{\text{QM matrix element}} e^{-\beta E_N^n}. \tag{24}$$

Notice how the temperature, T only appears in the last factor in (24). Let us now consider the ground state ($n = 0$) in the low temperature limit with energy E_0 corresponding to the state $|\psi_N\rangle_0$.

$$\begin{aligned}
\left\langle \hat{O} \right\rangle &\simeq \frac{1}{Z_{\beta=\infty}} e^{-\beta E_0} {}_0 \langle \psi_N | \hat{O} | \psi_N \rangle_0 \\
&= \frac{e^{-\beta E_0}}{e^{-\beta E_0}} {}_0 \langle \psi_N | \hat{O} | \psi_N \rangle_0,
\end{aligned}$$

such that

$$\left\langle \hat{O} \right\rangle \overset{\beta \to \infty}{=} {}_0 \langle \psi_N | \hat{O} | \psi_N \rangle_0. \tag{25}$$

We now have a way to calculate the statistical mean value in the ground state at zero temperature. Let us now now assume that the energy spectrum

is such that the ground state is separated from excited states by a <u>gap</u> (band insulators, semiconductors, superconductors). This way, we can express the excited state energies as

$$E_N^1 = E_N^0 + \Delta_N \tag{26}$$

such that

$$E_N^2, E_N^3, \cdots \geq E_N^1. \tag{27}$$

This way, we get from (24)

$$
\begin{aligned}
\left\langle \hat{O} \right\rangle &= \frac{1}{Z} \sum_n {}_n \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_n \mathrm{e}^{-\beta E_N^n} \\
&= \frac{\sum_n {}_n \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_n \mathrm{e}^{-\beta E_N^n}}{\sum_n \mathrm{e}^{-\beta E_N^n}} \\
&= \cdots \\
&= \frac{{}_0 \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_0 \mathrm{e}^{-\beta E_N^0 \left(1 + \mathrm{e}^{-\beta \Delta} \cdots \right)}}{\mathrm{e}^{-\beta E_N^0} \left(1 + \mathrm{e}^{-\beta \Delta} \cdots \right)}
\end{aligned}
\tag{28}
$$

and we find that as $\beta \Delta \gg 1$, $\hat{O} \simeq {}_0 \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_0$. In semiconductors we find $\Delta \sim 10\mathrm{mev} \sim 1000\mathrm{K}$.

2 Coherent states and Grassman variables

Pages 10-17 in lecture notes.

2.1 Coherent states

A coherent state (both for fermions and bosons) is defined as an eigenstate to an annihilation operator

$$a_\mu \left|\phi\right\rangle = \varphi_\mu \left|\phi\right\rangle \qquad \textbf{Bosons} \qquad (29)$$

$$c_\mu \left|\psi\right\rangle = \xi_\mu \left|\psi\right\rangle \qquad \textbf{Fermions} \qquad (30)$$

Both $\left|\psi\right\rangle$ and $\left|\phi\right\rangle$ must contain a component with the least (≥ 0) quantum number (quant), but it is clear that neither $\left|\psi\right\rangle$ nor $\left|\phi\right\rangle$ can be states with a sharply defined number of particles. They are therefore also "hard to destroy". This also explains why we chose to define them as eigenstates of the annihilation operators, not the creation operators. We will get back to the creation of these coherent states.

We will first look at the bosonic case:

2.1.1 Bosonic case

$$a_\mu \left|\phi\right\rangle = \varphi_\mu \left|\phi\right\rangle \qquad (31)$$

$$[a_\mu, a_\nu] = 0$$
$$\Rightarrow (a_\mu a_\nu - a_\nu a_\mu) \left|\phi\right\rangle = 0$$
$$= (\varphi_\mu \varphi_\nu - \varphi_\nu \varphi_\mu) \left|\phi\right\rangle$$
$$\Rightarrow [\varphi_\mu, \varphi_\nu] = 0. \qquad (32)$$

Equation (32) will always be satisfied if $\varphi_\mu \in \mathbb{C}$. **The eigenvalues to coherent boson states can be chosen as complex numbers. This is something we can state without knowing anything about how these states are constructed.**

2.1.2 Fermionic case

$$c_\mu \left|\psi\right\rangle = \xi_\mu \left|\psi\right\rangle \qquad (33)$$

$$\{c_\mu, c_\nu\} = 0$$
$$\Rightarrow (c_\mu c_\nu + c_\nu c_\mu) \left|\psi\right\rangle = 0$$
$$= (\xi_\mu \xi_\nu + \xi_\nu \xi_\mu) \left|\psi\right\rangle$$
$$\Rightarrow \{\xi_\mu, \xi_\nu\} = 0. \qquad (34)$$

If $\xi_\mu \in \mathbb{C}$, (34) will only be satisfied if $\{\xi_\mu\} = 0$, trivial eigenvalues. **The eigenvalues for coherent fermion states must be chosen as anti-commuting numbers, Grassmann-variables.**

2.2 Grassmann variables

2.2.1 Fundamentals

Equation (34) states the fundamental property of Grassmann variables, and it immediately follows that

$$\xi_\mu^2 = 0, \tag{35}$$

the squares of the Grassmann variables vanish! Similarly we have that $\xi^n = \xi^2 \xi^{n-2} = 0, n \geq 2$. An arbitrary series expansion in Grassmann variables

$$f(\xi) = \sum_n c_n \xi^n$$
$$= c_0 + c_1 \xi + \dots$$
$$= c_0 + c_1 \xi \tag{36}$$

is linear. We can also consider $f(\xi^*) = c_0 + c_1 \xi^*$, where $(\xi^*)^* = \xi$. An arbitrary function of ξ, ξ^* can be written on the forms

$$A(\xi, \xi^*) = c_0 + c_1 \xi + c_2 \xi^* + c_3 \xi \xi^* \tag{37}$$
$$= c_0 + c_1 \xi + c_2 \xi^* + d_3 \xi^* \xi \tag{38}$$

We will now look into some of the properties of functions of Grassmann variables.

2.2.2 Differentiation

Differentiation with respect to Grassman variables follows

$$\frac{\partial \xi}{\partial \xi} = 1 \qquad\qquad \frac{\partial \xi}{\partial \xi^*} = 0 \tag{39}$$

$$\frac{\partial \xi^*}{\partial \xi} = 0 \qquad\qquad \frac{\partial \xi^*}{\partial \xi^*} = 1 \tag{40}$$

$$\frac{\partial (\xi \xi^*)}{\partial \xi} = \xi^* \tag{41}$$

$$\frac{\partial (\xi \xi^*)}{\partial \xi^*} = -\frac{\partial (\xi^* \xi)}{\partial \xi^*} = -\xi \tag{42}$$

$$\frac{\partial f(\xi)}{\partial \xi^*} = 0 \tag{43}$$

$$\frac{\partial f(\xi)}{\partial \xi} = c_1 = \frac{\partial f(\xi^*)}{\partial \xi^*}, \tag{44}$$

and for functions defined as in (37), we have

$$\frac{\partial}{\partial \xi} A\left(\xi, \xi^*\right) = c_1 + c_3 \xi^* = c_1 - d_3 \xi^* \tag{45}$$

$$\frac{\partial}{\partial \xi^*} A\left(\xi, \xi^*\right) = c_2 - c_3 \xi = c_2 + d_3 \xi. \tag{46}$$

2.2.3 Integration

Integrating with respect to Grassmann variables are motivated from the properties of "normal" Riemann integrals, that if $f\left(x = \pm \infty\right)$, then

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{\mathrm{d}f}{\mathrm{d}x} = 0. \tag{47}$$

Equivalently we define

$$\int \mathrm{d}\xi \cdot 1 = \int \mathrm{d}\xi \, \frac{\mathrm{d}\xi}{\mathrm{d}\xi} = 0 \tag{48}$$

$$\int \mathrm{d}\xi^* = 0, \tag{49}$$

in other words, the integral of a total differential is zero.

$$\int \mathrm{d}\xi \, \xi = \int \mathrm{d}\xi^* \, \xi^* = 1 \tag{50}$$

is a "normalization" criteria. These relations define what we mean by Grassmann-integration.

Now, we have

$$\int \mathrm{d}\xi \, f\left(\xi\right) = c_1 \tag{51}$$

$$\frac{\partial f}{\partial \xi} = c_1 \tag{52}$$

$$\int \mathrm{d}\xi \, A\left(\xi, \xi^*\right) = \int \mathrm{d}\xi \left(x_0 + c_1 \xi + c_2 \xi^* + c_3 \xi \xi^*\right)$$
$$= c_1 + c_3 \xi^*. \tag{53}$$

As we can see by comparing (53) with (45), "integration" = "derivation". The somewhat hand wavy definition of integration is motivated by the fact that it gives results that reminds us about results from the theory for complex functions.

2.2.4 The number operator

Generally, we have that

$$a^\dagger_\mu \left|\phi\right\rangle \neq \left|\phi\right\rangle \qquad\qquad c^\dagger_\mu \left|\xi\right\rangle \neq \left|\xi\right\rangle, \qquad\qquad (54)$$

and so

$$a^\dagger_\mu a_\mu \left|\phi\right\rangle \neq N^\phi_\mu \left|\phi\right\rangle \qquad\qquad (55)$$

$$c^\dagger_\mu c_\mu \left|\xi\right\rangle \neq N^\xi_\mu \left|\xi\right\rangle. \qquad\qquad (56)$$

The coherent states are <u>not</u> eigenstates of the counting operator. $\left|\phi\right\rangle, \left|\xi\right\rangle$ are not states with a fixed number of "quants".

2.2.5 Algebra

Consider a vector space with the following additional properties:

1) $$(xy)z = x(yz)$$
2) $$x(y+z) = xy + xz$$
3) $$(x+y)z = xz + yz$$
4) $$\alpha xy = x\alpha y.$$

In Abelian algebra, $xy = yx$, while in Grassmann algebra $xy = -yx$. <u>Complex numbers</u> are generators for the Abelian algebra over the field $\mathbb{G}$ of commuting numbers. <u>Grassmann numbers</u> are generators for the algebra over the field $\mathbb{G}$ of anticommuting numbers.

3 Coherent states for bosons

4 Coherent states for fermions

5 Gaussian integrals

6   Matsubara sums and contour integrals

7   Feynman path integrals

8 Imaginary time path integrals and the partition function

9 The partition function for a free electron gas

10 Functional integrals over quantum fields

11 Coherent states path integral