TFY4210, Quantum theory of many-particle systems, 2016: Solution to Tutorial 1

1. Many-particle wavefunctions.

(i) Since we are dealing with fermions, $\xi = -1$. Let's assume that our chosen ordering of the states in the single-particle basis set $\{\nu\}$ is such that $\nu_1 < \nu_2 < \nu_3$. Then

$$\Phi_{\nu_1,\nu_2,\nu_3}(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}} \sum_{P\in S_3} (-1)^{t_P} \cdot P\phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2)\phi_{\nu_3}(x_3). \tag{1}$$

There are $3! = 6$ permutations of the starting list (ν_1,ν_2,ν_3). They are given in the table below, together with examples of the product of transpositions P_{jk} used to obtain them from the starting list (recall that P_{jk} permutes the entries in positions j and k in the list). For example, the fourth permutation in the table can be written $P_{13}P_{12}(\nu_1,\nu_2,\nu_3) = P_{13}(\nu_2,\nu_1,\nu_3) = (\nu_3,\nu_1,\nu_2)$.

P	Product of transpositions	t_P	$(-1)^{t_P}$
(ν_1,ν_2,ν_3)		0	1
(ν_1,ν_3,ν_2)	P_{23}	1	-1
(ν_2,ν_1,ν_3)	P_{12}	1	-1
(ν_3,ν_1,ν_2)	$P_{13}P_{12}$	2	1
(ν_2,ν_3,ν_1)	$P_{12}P_{13}$	2	1
(ν_3,ν_2,ν_1)	P_{13}	1	-1

From the table we see that Eq. (1) becomes

$$\begin{aligned}\Phi_{\nu_1,\nu_2,\nu_3}(x_1,x_2,x_3) &= \frac{1}{\sqrt{3!}}[\phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2)\phi_{\nu_3}(x_3) - \phi_{\nu_1}(x_1)\phi_{\nu_3}(x_2)\phi_{\nu_2}(x_3) \\ &- \phi_{\nu_2}(x_1)\phi_{\nu_1}(x_2)\phi_{\nu_3}(x_3) + \phi_{\nu_3}(x_1)\phi_{\nu_1}(x_2)\phi_{\nu_2}(x_3) \\ &+ \phi_{\nu_2}(x_1)\phi_{\nu_3}(x_2)\phi_{\nu_1}(x_3) - \phi_{\nu_3}(x_1)\phi_{\nu_2}(x_2)\phi_{\nu_1}(x_3)]. \end{aligned} \tag{2}$$

You can verify that this expression can be written as a determinant:

$$\Phi_{\nu_1,\nu_2,\nu_3}(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \phi_{\nu_1}(x_2) & \phi_{\nu_1}(x_3) \\ \phi_{\nu_2}(x_1) & \phi_{\nu_2}(x_2) & \phi_{\nu_2}(x_3) \\ \phi_{\nu_3}(x_1) & \phi_{\nu_3}(x_2) & \phi_{\nu_3}(x_3) \end{vmatrix} \tag{3}$$

(ii) For this question the determinant form (3) is convenient. We use the following properties of the determinant of a matrix: if two columns are interchanged, or if two rows are interchanged, the determinant changes sign. Interchanging x_1 and x_2 in (3) corresponds to interchanging columns 1 and 2 in the matrix, hence Φ changes sign. Next, take two of the single-particle states to be identical, e.g. ν_1 and ν_2. This means that rows 1 and 2 of the matrix become identical. Interchanging these rows thus has no effect on the matrix, but the determinant must change sign. Hence $\det|\ldots| = -\det|\ldots|$, which implies $\det|\ldots| = 0$.

(iii) To avoid unnecessary clutter in some of the expressions that follow, define $C \equiv \frac{1}{\sqrt{N!}\sqrt{\prod_\nu n_\nu!}}$. We get

$$\begin{aligned}\hat{O}\Phi_{\nu_1,\nu_2,\ldots,\nu_N}(x_1, x_2, \ldots, x_N) &= \left(\sum_{i=1}^{N} \hat{o}_i\right) \Phi_{\nu_1,\nu_2,\ldots,\nu_N}(x_1, x_2, \ldots, x_N) \\ &= C \sum_{P\in S_N} \xi^{t_P} \left(\sum_{i=1}^{N} \hat{o}_i\right) \phi_{P\nu_1}(x_1)\phi_{P\nu_2}(x_2)\ldots\phi_{P\nu_N}(x_N). \quad (4)\end{aligned}$$

Here $(P\nu_1, P\nu_2, \ldots, P\nu_N)$ defines the permutation P of the starting list $(\nu_1, \nu_2, \ldots, \nu_N)$. The operator $\hat{o}_i$ only involves the coordinates x_i. For example, a common situation/choice is that $\hat{o}_i = -\frac{\hbar^2}{2m}\nabla_i^2 + u(x_i)$, where $u(x)$ is some external potential (which could be 0). Using the eigenvalue equation

$$\hat{o}_i\phi_\nu(x_i) = o_\nu\phi_\nu(x_i) \quad (5)$$

gives

$$\hat{O}\Phi_{\nu_1,\nu_2,\ldots,\nu_N}(x_1, x_2, \ldots, x_N) = C \sum_{P\in S_N} \xi^{t_P} \left(\sum_{i=1}^{N} o_{P\nu_i}\right) \phi_{P\nu_1}(x_1)\phi_{P\nu_2}(x_2)\ldots\phi_{P\nu_N}(x_N). \quad (6)$$

Now note that the sum of the eigenvalues is independent of the permutation P:

$$\sum_{i=1}^{N} o_{P\nu_i} = o_{P\nu_1} + o_{P\nu_2} + \ldots + o_{P\nu_N} = \sum_\nu o_\nu n_\nu \quad (7)$$

where (as before) n_ν is the number of particles in the single-particle state ν in the many-particle state $\Phi_{\nu_1,\nu_2,\ldots,\nu_N}$ (i.e. n_ν is the number of times the function ϕ_ν appears in each term in $\Phi_{\nu_1,\nu_2,\ldots,\nu_N}$). This sum can therefore be moved outside the sum over P, giving the desired result:

$$\hat{O}\Phi_{\nu_1,\nu_2,\ldots,\nu_N} = \left(\sum_\nu o_\nu n_\nu\right) \Phi_{\nu_1,\nu_2,\ldots,\nu_N}. \quad (8)$$

2. Fermionic creation and annihilation operators.

(a)

$$c_3c_2^\dagger|1_1, 0_2, 1_3, \ldots\rangle = -c_3|1_1, 1_2, 1_3, \ldots\rangle = -(-1)^2|1_1, 1_2, 0_3, \ldots\rangle = -|1_1, 1_2, 0_3, \ldots\rangle. \quad (9)$$

(b) We have

$$c_\nu|n\rangle = (-1)^{\sum_{\rho<\nu} n_\rho} n_\nu|n_1, \ldots, 0_\nu, \ldots\rangle, \quad (10)$$

so

$$\langle \bar{n}|c_\nu|n\rangle = (-1)^{\sum_{\rho<\nu} n_\rho} n_\nu \langle \bar{n}|n_1, \ldots, 0_\nu, \ldots\rangle = (-1)^{\sum_{\rho<\nu} n_\rho} n_\nu \delta_{\bar{n}_\nu,0} \prod_{\rho\neq\nu} \delta_{n_\rho,\bar{n}_\rho}. \tag{11}$$

On the other hand,

$$c_\nu^\dagger|\bar{n}\rangle = (-1)^{\sum_{\rho<\nu} \bar{n}_\rho}(1-\bar{n}_\nu)|\bar{n}_1, \ldots, 1_\nu, \ldots\rangle, \tag{12}$$

so

$$\langle n|c_\nu^\dagger|\bar{n}\rangle^* = (-1)^{\sum_{\rho<\nu} \bar{n}_\rho}(1-\bar{n}_\nu)\langle n|\bar{n}_1, \ldots, 1_\nu, \ldots\rangle = (-1)^{\sum_{\rho<\nu} \bar{n}_\rho}(1-\bar{n}_\nu)\delta_{n_\nu,1} \prod_{\rho\neq\nu} \delta_{n_\rho,\bar{n}_\rho} \tag{13}$$

(since the matrix element is real, taking the complex conjugate has no effect). The product $\prod_{\rho\neq\nu} \delta_{n_\rho,\bar{n}_\rho}$ is common to both (11) and (13), and implies that the exponent to which -1 is raised is the same in both expressions. Furthermore, since n_ν and $\bar{n}_\nu$ can only take the values 0 or 1, it follows that $\delta_{\bar{n}_\nu,0} = 1-\bar{n}_\nu$ and $\delta_{n_\nu,1} = n_\nu$. So (11) and (13) are identical. QED.

(c) It suffices to show that $\{c_\mu, c_\nu^\dagger\}|n\rangle = \delta_{\mu,\nu}|n\rangle$ where $|n\rangle$ is an arbitrary basis state. First consider $\mu = \nu$. We have

$$\begin{aligned} c_\nu c_\nu^\dagger|n\rangle &= (-1)^{\sum_{\rho<\nu} n_\rho}(1-n_\nu)c_\nu|\ldots, 1_\nu, \ldots\rangle = \underbrace{\left[(-1)^{\sum_{\rho<\nu} n_\rho}\right]^2}_{\mathrm{sign}^2=1}(1-n_\nu)\cdot 1|\ldots, 0_\nu, \ldots\rangle \\ &= (1-n_\nu)|n\rangle, \end{aligned} \tag{14}$$

where in the last line we replaced $|\ldots, 0_\nu, \ldots\rangle$ by $|n\rangle$, which is valid also for $n_\nu = 1$ since then the prefactor $1-n_\nu$ makes the expression vanish. Furthermore,

$$c_\nu^\dagger c_\nu|n\rangle = n_\nu|n\rangle \tag{15}$$

since $c_\nu^\dagger c_\nu$ is the number operator. So

$$(c_\nu c_\nu^\dagger + c_\nu^\dagger c_\nu)|n\rangle = (1-n_\nu+n_\nu)|n\rangle = |n\rangle = 1\cdot|n\rangle. \tag{16}$$

For $\mu < \nu$ we have

$$\begin{aligned} c_\mu c_\nu^\dagger|n\rangle &= (-1)^{\sum_{\rho<\nu} n_\rho}(1-n_\nu)c_\mu|\ldots, n_\mu, \ldots, 1_\nu, \ldots\rangle \\ &= (-1)^{\sum_{\rho<\nu} n_\rho + \sum_{\rho<\mu} n_\rho}(1-n_\nu)n_\mu|\ldots, 0_\mu, \ldots, 1_\nu, \ldots\rangle \end{aligned} \tag{17}$$

and

$$\begin{aligned} c_\nu^\dagger c_\mu|n\rangle &= (-1)^{\sum_{\rho<\mu} n_\rho} n_\mu c_\nu^\dagger|\ldots, 0_\mu, \ldots, n_\nu, \ldots\rangle \\ &= (-1)^{\sum_{\rho<\mu} n_\rho + \sum_{\rho<\nu} n_\rho + (0-n_\mu)} n_\mu(1-n_\nu)|\ldots, 0_\mu, \ldots, 1_\nu, \ldots\rangle. \end{aligned} \tag{18}$$

So

$$(c_\mu c_\nu^\dagger + c_\nu^\dagger c_\mu)|n\rangle = [1+(-1)^{n_\mu}]\,(-1)^{\sum_{\rho<\nu} n_\rho + \sum_{\rho<\mu} n_\rho} n_\mu(1-n_\nu)|\ldots, 0_\mu, \ldots, 1_\nu, \ldots\rangle. \tag{19}$$

If $n_\mu = 0$ the rhs is 0 because of the factor n_μ. If $n_\mu = 1$ the rhs is 0 because of the factor $[1 + (-1)^{n_\mu}]$. Since these are the only values n_μ can take, the rhs is 0 always, and we can write

$$(c_\mu c_\nu^\dagger + c_\nu^\dagger c_\mu)|n\rangle = 0 = 0 \cdot |n\rangle \quad (\mu < \nu). \tag{20}$$

One can show that the same result is obtained if $\mu > \nu$. So it follows that $\{c_\mu, c_\nu^\dagger\} = \delta_{\mu,\nu}$. QED.

(d) We have

$$\hat{n}_\nu^2 = \hat{n}_\nu \hat{n}_\nu = c_\nu^\dagger \underbrace{c_\nu c_\nu^\dagger}_{1 - c_\nu^\dagger c_\nu} c_\nu = c_\nu^\dagger c_\nu - \underbrace{c_\nu^\dagger c_\nu^\dagger}_{0} c_\nu c_\nu = \hat{n}_\nu. \quad \text{QED.} \tag{21}$$

That $(c_\nu^\dagger)^2 = 0$ follows from setting $\mu = \nu$ in $\{c_\mu^\dagger, c_\nu^\dagger\} = 0$. (Of course, we could instead have invoked the adjoint relation $(c_\nu)^2 = 0$.) Since $\hat{n}_\nu^2 = \hat{n}_\nu$, the corresponding relation also has to hold for the eigenvalues n_ν, i.e. $n_\nu^2 = n_\nu$. The solutions to this equation are $n_\nu = 0$ and $n_\nu = 1$ which therefore are the possible eigenvalues of $\hat{n}_\nu$.

2. Some useful commutator expressions.

(a) We have (with $\zeta = \pm 1$)

$$\begin{aligned} A[B,C]_\zeta - \zeta[A,C]_\zeta B &= A(BC + \zeta CB) - \zeta(AC + \zeta CA)B \\ &= ABC + \underbrace{\zeta ACB - \zeta ACB}_{0} - \underbrace{\zeta^2}_{1} CAB \\ &= [AB, C]. \end{aligned} \tag{22}$$

(b) Using Eq. (22) we get (with $\zeta = \pm 1$ for fermionic/bosonic operators, respectively)

$$[\hat{n}_\mu, c_\nu^\dagger] = [c_\mu^\dagger c_\mu, c_\nu^\dagger] = c_\mu^\dagger \underbrace{[c_\mu, c_\nu^\dagger]_\zeta}_{\delta_{\mu\nu}} - \zeta \underbrace{[c_\mu^\dagger, c_\nu^\dagger]_\zeta}_{0} c_\mu = \delta_{\mu\nu}\, c_\mu^\dagger, \tag{23}$$

$$[\hat{n}_\mu, c_\nu] = [c_\mu^\dagger c_\mu, c_\nu] = c_\mu^\dagger \underbrace{[c_\mu, c_\nu]_\zeta}_{0} - \zeta \underbrace{[c_\mu^\dagger, c_\nu]_\zeta}_{\zeta\delta_{\mu\nu}} c_\mu = -\delta_{\mu\nu}\, c_\mu. \tag{24}$$

In the last expression we used that $[c_\mu^\dagger, c_\nu]_\zeta = \zeta[c_\nu, c_\mu^\dagger]$, which follows from the general result

$$[B, A]_\zeta = \zeta[A, B]_\zeta. \tag{25}$$

(Proof: $[B,A]_\zeta = BA + \zeta AB = \zeta(\zeta BA + AB) = \zeta[A,B]_\zeta$.)