

## HW IV

Problem 1 (Courtesy Edward Groth, Princeton)

~~Consider a particle in a box~~ provides Aluminarios

The single-particle wavefunctions are of the form

$$|n_a, n_b\rangle = \sqrt{\frac{4}{ab}} \sin\left(\frac{\pi n_a x}{a}\right) \sin\left(\frac{\pi n_b y}{b}\right) \quad n_a, n_b > 0$$

and the energies are given by

$$E_{n_a, n_b} = \frac{\hbar^2 \pi^2}{2m} \left[ \left(\frac{n_a}{a}\right)^2 + \left(\frac{n_b}{b}\right)^2 \right]$$

The lowest-energy single particle state is  $|1, 1\rangle$  with energy

$$E_{11} = \frac{\hbar^2 \pi^2}{2m} \left[ \left(\frac{1}{a}\right)^2 + \left(\frac{1}{b}\right)^2 \right]$$

Since  $b$  is the largest side of the box, the next-lowest-energy state is  $|1, 2\rangle$  with energy

$$E_{12} = \frac{\hbar^2 \pi^2}{2m} \left[ \left(\frac{1}{a}\right)^2 + \left(\frac{2}{b}\right)^2 \right]$$

We write two-particle states as

$$|n_a^1, n_b^1\rangle |n_a^2, n_b^2\rangle$$

(c) Two distinguishable particles

Each particle can be placed in the lowest-energy single particle state, which is

$$\psi = |1, 1\rangle |1, 1\rangle$$

with energy

$$E_{1111} = 2 \frac{\hbar^2 \pi^2}{2m} \left[ \left(\frac{1}{a}\right)^2 + \left(\frac{1}{b}\right)^2 \right]$$

Now, to take the "contact interaction"  $V = ab V_0 \delta^2(\vec{r}_1 - \vec{r}_2)$  into account, we need the product of two integrals  $A_x A_y$  of the form

$$A_x = \frac{4}{a^2} \int_0^a dx_1 \int_0^a dx_2 \sin^2\left(\frac{\pi n_1^1 x_1}{a}\right) \sin^2\left(\frac{\pi n_1^2 x_2}{a}\right) \delta(x_1 - x_2)$$

$$= \frac{4}{a} \int_0^a dx \sin^2\left(\frac{\pi n_1^1 x}{a}\right) \sin^2\left(\frac{\pi n_1^2 x}{a}\right)$$

$$= 1 + \frac{1}{2} \delta_{n_1^1, n_1^2}$$

For the distinguishable case,  $n_a^1 = n_a^2 = 1$  and the integral is  $3/2$ . Putting this all together, we find

$$\Delta E = V_0 (A_x A_y) = V_0 (A_x)^2 = \frac{9}{4} V_0$$

(b) Two identical bosons

In this case, we have the added constraint that the wavefunction must be symmetric under the exchange of the two particles. But the state  $|1,1\rangle|1,1\rangle$  is just that, so no difference in the state, energy, or contact interaction energy relative to that of part (a).

(c) Identical spin- $\frac{1}{2}$  fermions in the singlet state

In this case the total wavefunction

$$\psi = \psi_{\text{space}} \psi_{\text{spin}}$$

must be antisymmetric. But the spin singlet wavefunction

$$\psi_{\text{spin}} = \frac{1}{\sqrt{2}} [|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle]$$

is itself antisymmetric, so the total wavefunction

$$\psi_{\text{tot}} = \psi_{\text{space}} \psi_{\text{spin}} = [ |1,1\rangle|1,1\rangle ] \frac{1}{\sqrt{2}} [ |\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle ]$$

is indeed antisymmetric under particle exchange. So again, no difference relative to (a).

(d) Identical spin- $\frac{1}{2}$  fermions in the triplet state.

In this case  $\Psi_{\text{spin}}$  is symmetric so  $\Psi_{\text{space}}$  must be antisymmetric. Our lowest-energy state is thus

$$\Psi = \frac{1}{\sqrt{2}} [ |1,1\rangle |1,2\rangle - |1,2\rangle |1,1\rangle ]$$

with energy

$$E_{1112} = E_{11} + E_{12} = \frac{\hbar^2 \pi^2}{2m} \left[ 2 \left( \frac{1}{a} \right)^2 + 5 \left( \frac{1}{b} \right)^2 \right]$$

Finally, we need the matrix element of the perturbation for this state. Note that

$$\Delta V = \frac{4}{b^2} \frac{1}{2} \int_0^b dy_1 \int_0^b dy_2 \left[ \sin\left(\frac{\pi y_1}{b}\right) \sin\left(\frac{2\pi y_2}{b}\right) - \sin\left(\frac{2\pi y_1}{b}\right) \sin\left(\frac{\pi y_2}{b}\right) \right]^2 \delta(y_1 - y_2)$$

$$= \frac{2}{\pi} \int_0^{\pi} dy \left[ \sin y \sin 2y - \sin 2y \sin y \right] = 0$$

Not surprisingly, the particles in the triplet state are prevented from being at the same place by the Pauli exclusion principle, so the contact interaction is 0.

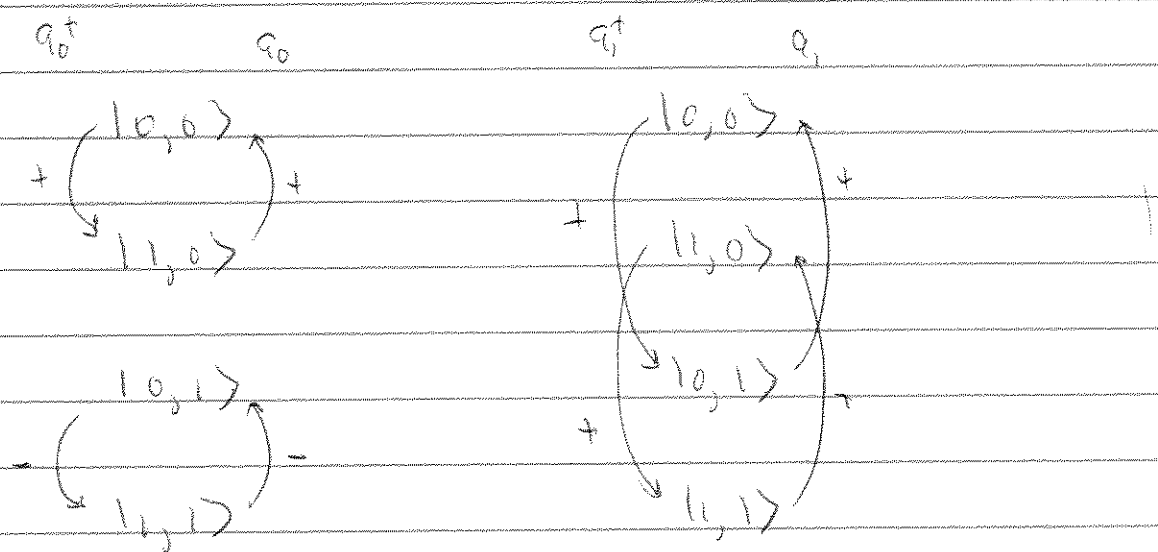
## Problem 2 (Baym 19.1)

In the nomenclature  $|n_0, n_1\rangle$ , let's choose the basis

$$|0,0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |0,1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |1,1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We need to use a bit of caution with respect to signs, c.f. p 415 of Baym, which are set to establish the proper exchange symmetry for fermions.

Below, we indicate the actions of  $a_0^\dagger, a_0, a_1^\dagger, a_1$  on the basis states, showing the correct relative signs. Note that we arbitrarily associate the "-" signs associated with filling and depleting the  $|1,1\rangle$  state w/ the first level; we presumably could have chosen the second level instead and gotten the same results.



This then gives us the following four matrices (you can easily verify!)

$$q_0 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad q_0^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$q_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad q_1^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

We are asked to check the anticommutation relations

$$\{a_0, a_0^\dagger\} \quad \{a_1, a_1^\dagger\} \quad \{a_0, a_1\} \quad \{a_0, a_1^\dagger\}$$

$$a_0 a_0^\dagger + a_0^\dagger a_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \mathbb{1}_4 \checkmark$$

$$a_1 a_1^\dagger + a_1^\dagger a_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \mathbb{1}_4 \checkmark$$

$$a_0 a_1 + a_1 a_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = 0 \quad \checkmark$$

$$a_0 a_1^t + a_1^t a_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = 0 \quad \checkmark$$

and so on...

### Problem 3

We have, from the second expression,

$$N = \sum_{\lambda} \int d^3r \varphi_{\lambda}^{\dagger}(\vec{r}) \varphi_{\lambda}(\vec{r}) \quad \text{making use of the definitions of the field operators}$$

$$= \sum_{\lambda} \int d^3r \sum_{\vec{p}} \frac{e^{-i(\vec{p} \cdot \vec{r})}}{\sqrt{V}} a_{\vec{p}, \lambda}^{\dagger} \sum_{\vec{p}'} \frac{e^{i(\vec{p}' \cdot \vec{r})}}{\sqrt{V}} a_{\vec{p}', \lambda}$$

$$= \sum_{\lambda} \sum_{\vec{p}, \vec{p}'} a_{\vec{p}, \lambda}^{\dagger} a_{\vec{p}', \lambda} \int d^3r \frac{e^{i(\vec{p}' - \vec{p}) \cdot \vec{r}}}{(V)^2}$$

The integral over  $r$  is just  $\delta(\vec{p} - \vec{p}')$ , whence

$$N = \sum_{\vec{p}, \lambda} a_{\vec{p}, \lambda}^{\dagger} a_{\vec{p}, \lambda}$$

and so it's shown.



### Problem 4

The guideline we seek is provided on pp. 425-426 of Baym. In one dimension, we have for particles of spin  $s$

$$G_s(x-x') = \langle \bar{\Psi}_0 | \psi_s^\dagger(x) \psi_s(x') | \bar{\Psi}_0 \rangle$$

where  $\bar{\Psi}_0$  is the  $T=0$  ground state of the Fermi gas, which is fully occupied, for each spin, for all states up to the Fermi level  $p_F$ .

Now,  $\psi_s(x) = \frac{1}{\sqrt{L}} \sum_p e^{ipx} a_{ps}$ , where we find that

$$G_s(x-x') = \frac{1}{L} \sum_{pp'} e^{-ipx} e^{ip'x'} \langle \bar{\Psi}_0 | a_{ps}^\dagger a_{p's} | \bar{\Psi}_0 \rangle$$

$$= \frac{1}{L} \sum_{p,p'} e^{-ipx} e^{ip'x'} \delta_{pp'} n_{ps}$$

$$= \frac{1}{L} \sum_p e^{-ip(x-x')} n_{ps}$$

$$\text{But, } n_{ps} = \begin{cases} 1 & -p_F \leq p \leq p_F \\ 0 & |p| > p_F \end{cases}$$

For a  $T=0$  Fermi gas, so for periodic boundary conditions in a 1-D box of length  $L$ ,

$$G_s(x-x') = \frac{1}{L} \sum_{p_f} e^{-ip(x-x')} = \frac{1}{L} \sum_{n=1}^{N_f} e^{-ip(x-x')}$$

where  $N_f = \frac{L p_f}{2\pi\hbar} = \frac{N_s}{2}$  with  $N_s$  the total number of fermions of spin  $s$  in the gas.

Note that, due to this relation by the way, the density

$$\rho = \frac{N}{L} = \frac{2N_s}{L} = \frac{4L p_f}{2\pi\hbar L} = \frac{2 p_f}{\pi\hbar} \quad (1)$$

Now, we note that the spacing between states in the Fermi gas (box) is

$$\Delta p = \frac{2\pi\hbar}{L}$$

so converting the sum over  $p$  into an integral over  $dp$ ,

$$G_s(x-x') \rightarrow \frac{1}{L} \left( \frac{L}{2\pi\hbar} \right) \int_{-p_f}^{p_f} e^{-ip(x-x')} dp$$

$$= \frac{1}{2\pi\hbar} \left\{ \int_{-p_f}^0 e^{-ip(x-x')} dp + \int_0^{p_f} e^{-ip(x-x')} dp \right\}$$

$$= \frac{1}{2\pi\hbar} \frac{1}{i\Delta} \left\{ 1 - e^{ip_f\Delta} + e^{-ip_f\Delta} - 1 \right\}$$

When we have defined  $\Delta = x - x'$ . Following through,

$$G_s(x-x') = \frac{1}{2\pi\hbar\Delta} \frac{1}{i} \left\{ e^{ip_F A} - e^{-ip_F A} \right\}$$

$$= \frac{\sin p_F A}{\pi\hbar\Delta}$$

If we now let  $z \equiv p_F A = p_F(x-x')$ , we find

$$G_s(x-x') = \frac{p_F}{\pi\hbar} \frac{\sin z}{z} = \frac{\rho}{2} \frac{\sin z}{z}$$

when  $\rho$  is the gas density, by (1) above. Substituting in the explicit form for  $z$ ,

$$G_s(x-x') = \frac{\rho}{2} \frac{\sin [p_F(x-x')]}{p_F(x-x')}$$

This function seems to me to be an effective "coherence length" of the influence of a particle of spin  $s$  at a position  $x'$  on a particle of the same spin at a distance  $x-x'$  away due to the influence of the Pauli exclusion principle.

## Problem 5 (Baym Problem 19.4)

The box needs to be multidimensional or the angular diverges (I found this out the hard way). So let's let it be a 3D box. Also, let the states be labelled  $\vec{p}_1 s_1$  and  $\vec{p}_2 s_2$ . We'll only consider the case  $\vec{p}_1 \neq \vec{p}_2$  since otherwise the parallel (equal) spin configuration is not allowed and the answer is indeterminate.

So, our state is

$$|E\rangle = |\vec{p}_1 s_1, \vec{p}_2 s_2\rangle$$

with  $\vec{p}_1 \neq \vec{p}_2$ , and will explore the difference between  $s_1 = s_2$  and  $s_1 \neq s_2$ .

From p434 of Baym, or class notes, we know that the interaction energy operator is given by

$$V = \frac{1}{2} \sum_{s_1 s_2} \int d^3 r_1 d^3 r_2 V(\vec{r}_1 - \vec{r}_2) \psi_{s_1}^+(\vec{r}_1) \psi_{s_2}^+(\vec{r}_2) \psi_{s_1}(\vec{r}_2) \psi_{s_2}(\vec{r}_1)$$

In the mean time, the field annihilation (creation) operator is given by

$$\psi_s^{(+)}(\vec{r}) = \sum_{\vec{p}} \frac{e^{i(\vec{p} \cdot \vec{r})}}{\sqrt{V}} a_{\vec{p}, s}^{(+)}$$

Taking the expectation value of  $V$  for our state  $|E\rangle$ , and using this expression for the field operators, we find that (writing for shorthand  $\vec{p} \cdot \vec{r} = pr$ )

$$V = \langle I | V_{op} | I \rangle =$$

$$= \frac{1}{2} \sum_{ss'} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \frac{1}{V^2} \sum_{pp'qq'} \left[ \langle I | e^{-i\vec{p}\cdot\vec{r}_1} e^{-i\vec{q}\cdot\vec{r}_2} e^{i\vec{q}'\cdot\vec{r}_2} e^{i\vec{p}'\cdot\vec{r}_1} \right. \\ \left. \times a_{p's}^+ a_{q's'}^+ a_{q's} a_{p's'} | I \rangle \right]$$

$$= \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \sum_{ss'pp'qq'} e^{-i(\vec{p}-\vec{p}')\cdot\vec{r}_1} e^{-i(\vec{q}-\vec{q}')\cdot\vec{r}_2} \langle I | a_{p's}^+ a_{q's'}^+ a_{q's} a_{p's'} | I \rangle$$

$$\boxed{s_1 \neq s_2}$$

We have two cases to consider. First, we consider  $s_1 \neq s_2$ . The two possibilities are  $(s_1, s_2) = (+, -)$  and  $(-, +)$ , and we'll want the average of these two. But the interaction energy will be the same for both, so we just pick one or the other, this say  $(+, -)$ . This keeping this in mind we then note that when we remove a particle of momentum  $\vec{p}'$  and spin  $s$ , when we put the particle with spin  $s$  back into the state it will also need to have momentum  $\vec{p}'$ . So, similarly, for the oppositely spinning  $s'$  will need to be put back with whatever momentum it had when it was removed. Thus, when  $s \neq s'$

$$\vec{p} = \vec{p}' \quad \vec{q} = \vec{q}'$$

is required.

Thus,

$$\bar{V}_{+-} = \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \sum_{s, s', p, p'} \delta_{pp'} \delta_{ss'} e^{-i(p-p')r_1 - i(q-q')r_2} \langle \mathbb{E} | a_{p's}^\dagger a_{q's'}^\dagger a_{q's} a_{p's} | \mathbb{E} \rangle$$

$$= \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \sum_{s, s', p, q} \langle \mathbb{E} | a_{p's}^\dagger a_{q's'}^\dagger a_{q's} a_{p's} | \mathbb{E} \rangle$$

Now, recalling that  $|\mathbb{E}\rangle = |\vec{p}_1, s_1, \vec{p}_2, s_2\rangle$ , then there are only two non-zero contributions from the sum over  $s, s', p, q$

$$\left. \begin{array}{l} \vec{p} = \vec{p}_1 \quad s = + \quad \vec{q} = \vec{p}_2 \quad s' = - \\ \vec{p} = \vec{p}_2 \quad s = - \quad \vec{q} = \vec{p}_1 \quad s' = + \end{array} \right\} \text{SO}$$

$$\bar{V}_{+-} = \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \left[ \langle \mathbb{E} | a_{p_1 s_1}^\dagger a_{p_2 s_2}^\dagger a_{p_2 s_2} a_{p_1 s_1} | \mathbb{E} \rangle + \langle \mathbb{E} | a_{p_2 s_2}^\dagger a_{p_1 s_1}^\dagger a_{p_1 s_1} a_{p_2 s_2} | \mathbb{E} \rangle \right]$$

But since  $\{a_{p's}, a_{p's'}^\dagger\} = 0$  for  $p's \neq p's'$ , and  $\{a_{p's}, a_{p's}\} = 0$  for any  $p's$ , then we can anticommute  $a_{p_1 s_1}^\dagger$  two places to the right in the first term, and  $a_{p_2 s_2}$  two places to the left in the second term, to get

$$\bar{V}_{+-} = \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \cdot 2 \left[ \langle \mathbb{E} | a_{p_2 s_2}^\dagger a_{p_2 s_2} a_{p_1 s_1}^\dagger a_{p_1 s_1} | \mathbb{E} \rangle \right] =$$

$$\frac{1}{V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \left[ \langle \mathbb{I} | n_{p_1 s_1} n_{p_2 s_2} | \mathbb{I} \rangle \right]$$

But since there is exactly one particle in each of the states  $p_1 s_1$  and  $p_2 s_2$ , the term in brackets is just 1, so

$$V_{+-} = \frac{1}{V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \quad (\text{A})$$

We hold off on evaluating this integral until later.

$$\boxed{s_1 = s_2}$$

For this, we want an average of  $++$  and  $--$ , but again they should be the same, so we choose  $++$  just to be definite.

We recall our general expression

$$V = \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \sum_{\text{supp } q, q'} e^{-i(p-p')r_1} e^{-i(q-q')r_2} \langle \mathbb{I} | a_{p_1}^\dagger a_{q_1}^\dagger a_{q_2} a_{p_2} | \mathbb{I} \rangle$$

First, we note that since  $s = s'$ , we now have

$$V_{++} = \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \sum_{\text{supp } q, q'} e^{-i(p-p')r_1} e^{-i(q-q')r_2} \langle \mathbb{I} | a_{p_1}^\dagger a_{q_1}^\dagger a_{q_2} a_{p_2} | \mathbb{I} \rangle$$

So if we remove a particle w/ momentum  $p'$  and replace it, again with  $p'$ , we can have either  $p = p'$  or  $q = p'$ . So we get two possibilities rather than one:

$$\vec{p}' = \vec{p} \quad \vec{q}' = \vec{q} \quad \text{as before}$$

$$\vec{p}' = \vec{q} \quad \vec{q}' = \vec{p} \quad \text{new term!}$$

Let's work on the inner product factor:

$$\begin{aligned} \langle \mathbb{E} | a_{\vec{p}}^{\dagger} a_{\vec{q}}^{\dagger} a_{\vec{q}} a_{\vec{p}} | \mathbb{E} \rangle &\rightarrow \delta_{\vec{p}\vec{p}} \delta_{\vec{q}\vec{q}} \langle \mathbb{E} | a_{\vec{p}}^{\dagger} a_{\vec{q}}^{\dagger} a_{\vec{q}} a_{\vec{p}} | \mathbb{E} \rangle + \\ &+ \delta_{\vec{p}\vec{q}} \delta_{\vec{q}\vec{p}} \langle \mathbb{E} | a_{\vec{p}}^{\dagger} a_{\vec{q}}^{\dagger} a_{\vec{p}} a_{\vec{q}} | \mathbb{E} \rangle \end{aligned}$$

Since by hypothesis  $p \neq q$  (remember we agreed for that at the very beginning of the problem), then we can anticommute the creation/annihilation operators to manipulate them into the form  $a_{\vec{p}}^{\dagger} a_{\vec{p}} a_{\vec{q}}^{\dagger} a_{\vec{q}} = n_{\vec{p}} n_{\vec{q}}$ . This involves two anticommutators (not "+" sign) for the first term, but only 1 anticommutator (not "-" sign) for the second term, so

$$\langle \mathbb{E} | a_{\vec{p}}^{\dagger} a_{\vec{q}}^{\dagger} a_{\vec{q}} a_{\vec{p}} | \mathbb{E} \rangle \rightarrow (\delta_{\vec{p}\vec{p}} \delta_{\vec{q}\vec{q}} - \delta_{\vec{p}\vec{q}} \delta_{\vec{q}\vec{p}}) \langle \mathbb{E} | n_{\vec{p}} n_{\vec{q}} | \mathbb{E} \rangle \text{ w/ so}$$

$$\begin{aligned} V_{++} &= \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2) \sum_{\vec{p}\vec{q}\vec{q}'\vec{p}'} \left[ \delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} \langle \mathbb{E} | n_{\vec{p}} n_{\vec{q}} | \mathbb{E} \rangle - \right. \\ &\quad \left. - \delta_{\vec{p}\vec{q}'} \delta_{\vec{q}\vec{p}'} e^{-i(\vec{p}\vec{q})r_1} e^{-i(\vec{q}-\vec{p})r_2} \langle \mathbb{E} | n_{\vec{p}} n_{\vec{q}} | \mathbb{E} \rangle \right] \end{aligned}$$

= being very pedantic here to avoid confusion

$$= \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2) \sum_{\vec{p}\vec{q}} \left[ \langle \mathbb{E} | n_{\vec{p}} n_{\vec{q}} | \mathbb{E} \rangle - e^{i(\vec{p}-\vec{q})(r_1-r_2)} \langle \mathbb{E} | n_{\vec{p}} n_{\vec{q}} | \mathbb{E} \rangle \right]$$

Now, our possibilities for  $\vec{p}, \vec{q}$  are



$$\left. \begin{array}{l} p = p_1, s = + \quad q = p_2, s = + \\ p = p_2, s = + \quad q = p_1, s = + \end{array} \right\} \text{so using these two possibilities,} \\ \text{we resolve the sums over } s, p, q \text{ and}$$

$$\sum_{s, p, q} \langle \mathbb{I} | n_{p_1} n_{q_1} | \mathbb{I} \rangle \rightarrow \langle \mathbb{I} | n_{p_1} n_{p_2} | \mathbb{I} \rangle + \langle \mathbb{I} | n_{p_2} n_{p_1} | \mathbb{I} \rangle = 2$$

$$\sum_{s, p, q} e^{-i(p-q)(r_1-r_2)} \langle \mathbb{I} | n_{p_1} n_{q_1} | \mathbb{I} \rangle \rightarrow$$

$$\rightarrow e^{-i(p_1-p_2)(r_1-r_2)} \langle \mathbb{I} | n_{p_1} n_{p_2} | \mathbb{I} \rangle + e^{-i(p_2-p_1)(r_1-r_2)} \langle \mathbb{I} | n_{p_2} n_{p_1} | \mathbb{I} \rangle$$

$$= e^{i(p_1-p_2)(r_1-r_2)} + e^{-i(p_1-p_2)(r_1-r_2)} = 2 \cos[(\vec{p}_1 - \vec{p}_2) \cdot (\vec{r}_1 - \vec{r}_2)]$$

putting the vector notation back into the dot product. So,

$$V_{++} \rightarrow \frac{1}{2V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \left[ 2 - 2 \cos[(\vec{p}_1 - \vec{p}_2) \cdot (\vec{r}_1 - \vec{r}_2)] \right]$$

(A)

(B)

$$= \frac{1}{V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) - \frac{1}{V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \cos[(\vec{p}_1 - \vec{p}_2) \cdot (\vec{r}_1 - \vec{r}_2)]$$

But, the (A) term on this page is identical to that on p.4, so,

$$V_{++} = V_{+-} = \frac{1}{V^2} \int d^3r_1 d^3r_2 V(\vec{r}_1 - \vec{r}_2) \cos[(\vec{p}_1 - \vec{p}_2) \cdot (\vec{r}_1 - \vec{r}_2)]$$

This integral, for  $V = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$ , is the answer we seek!

Pursuing this, we are simply asking to compute the "exchange energy"

$$V_X = \frac{1}{V^2} \int d^3r_1 d^3r_2 V(r_1 - r_2) \cos[(p_1 - p_2) \cdot (r_1 - r_2)]$$

$$= \frac{1}{V^2} \int d^3R d^3r V(r) \cos(\vec{\Delta} \cdot \vec{r})$$

where we have defined  $\vec{\Delta} \equiv \vec{p}_1 - \vec{p}_2$  and made the transformation

$$\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \quad \vec{r} = \vec{r}_1 - \vec{r}_2$$

Performing the  $R$  integral and substituting  $V(r) = e^2/r$ ,

$$V_X = \frac{e^2}{V} \int d^3r \frac{\cos(\vec{\Delta} \cdot \vec{r})}{r}$$

Now, wlog, we align the  $z$  axis with  $\vec{\Delta} = \vec{p}_1 - \vec{p}_2$  (energy can't depend on orientation of the axis), so  $\vec{\Delta} \cdot \vec{r} = \Delta r \cos\theta$ .

Performing the  $\phi$  integration (does that even do anything other than bring out a factor of  $2\pi$ , I ask you!?)

$$V_X = \frac{2\pi e^2}{V} \int_0^g \int_{-1}^1 \frac{r^2 dr d(\cos\theta)}{r} \cos(\Delta r \cos\theta) = \frac{2\pi e^2}{V} \int_0^g \int_{-1}^1 dr dz r \cos(\Delta r z)$$

where we have let " $g$ " be the radius of the sphere of volume  $V$ .

Continuing with the integration

$$V_x = \frac{2\pi e^2}{V} \int_0^R dr dz r \left[ \frac{\sin(\Delta r z)}{\Delta r} \right]$$

$$= \frac{4\pi e^2}{\Delta V} \int_0^R dr \sin(\Delta r)$$

Letting  $y = \Delta r$ , so  $dr = dy/\Delta$

$$r=R \Rightarrow y = \Delta R$$

$$= \frac{4\pi e^2}{\Delta^2 V} \int_0^{\Delta R} \sin y dy = \frac{4\pi e^2}{\Delta^2 V} [1 - \cos(\Delta R)]$$

Finally, recognizing that  $V = \frac{4}{3}\pi R^3$  is the volume of the sphere, and using  $1 - \cos \theta = 2\sin^2 \theta/2$ , we find the exchange energy

$$V_x = \frac{6e^2}{\Delta^2 R^3} \sin^2\left(\frac{\Delta R}{2}\right)$$

Finally, we make use of Bohr's  $x$  variable  $X = \Delta R$  to write

$$V_x = \frac{6e^2}{R X^2} \sin^2\left(\frac{X}{2}\right)$$