# LECTURES ON MANY BODY THEORY

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# LECTURE 1: SECOND QUANTIZATION - HARMONIC OSCILLATOR

## Consequences of indistinguishability

In quantum mechanics, identical particles are indistinguishable. In fact, even if we imagine that originally all particles are numbered, if we observe a particle at some place after a finite period of time, we cannot say with certainty which number it carries. This is because in quantum mechanics the notion of particle trajectory loses its sense.

Because of this fundamentally new property, the wavefunction of a two-particle system,  $\psi(1,2)$  (where 1 and 2 are the coordinates -including spin- of particles 1 and 2) should be physically equivalent to  $\psi(2,1)$ . This means the two wavefunctions may differ only by a phase factor:

$$\psi(1,2) = e^{i\phi}\psi(2,1) = e^{2i\phi}\psi(1,2),\tag{1}$$

where in the second equation we have used the same argument once more. This means in turn that  $e^{2i\phi} = 1$ , which can be realized in two ways: either  $e^{i\phi} = 1$  or  $e^{i\phi} = -1$ . It is an experimental fact that the first possibility is realized for particles with integer spin (bosons), while the second possibility is realized for particles with half-integer spin (fermions).

In condensed-matter physics, we consider electrons, protons, and neutrons as elementary particles. All of them have spin 1/2, i.e. they are fermions. So why do we speak about bosons? At not too high energies, bound states of electrons, protons, and nucleons can be considered as elementary. For instance, when dealing with liquid <sup>4</sup>He at cryogenic temperatures, we can safely neglect all the excited states of this atom. Now, since it consists of an even number of fermions (2e+2p+2n), an exchange of two helium atoms does not lead to a minus sign in the many body wavefunction, i.e. the atom <sup>4</sup>He is a boson. On the other hand, it is worth pointing out that the other stable isotope, <sup>3</sup>He, is a fermion, being composed of only five elementary particles (2e+2p+1n).

## Harmonic oscillator

Another type of bosonic excitations dealt with in condensed matter physics are quanta of various types of oscillations, like electromagnetic oscillations (the quantum, photon, has spin S = 1), or lattice vibrations (the quantum, phonon, carries integer spin). Let us therefore consider the simplest oscillator for the start, namely the harmonic oscillator with mass m and spring constant K, whose Hamiltonian reads

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2,$$
 (2)

where x is the coordinate and  $p = -i\hbar d/dx$  is the canonically conjugate momentum. Let us introduce the classical frequency  $\omega = \sqrt{K/m}$  and a dimensionless coordinate  $\xi = x\sqrt{m\omega/\hbar}$ . Then the Hamiltonian can be written in the form  $H = 2^{-1}\hbar\omega \left(-d^2/d\xi^2 + \xi^2\right)$ . Let us define furthermore the operators

$$a = \frac{1}{\sqrt{2}} \left( \xi + \frac{d}{d\xi} \right), \tag{3}$$

$$a^{\dagger} = \frac{1}{\sqrt{2}} \left( \xi - \frac{d}{d\xi} \right). \tag{4}$$

Note that  $a, a^{\dagger}$  are Hermitian conjugate operators. It is easy to show that the Hamiltonian can be written

$$H = \frac{\hbar\omega}{2} \left( a^{\dagger}a + aa^{\dagger} \right) = \hbar\omega \left( a^{\dagger}a + \frac{1}{2} \right).$$
(5)

In the second equation we have used the following commutation relation between the operators  $a, a^{\dagger}$ ,

$$[a, a^{\dagger}] = 1. \tag{6}$$

In order to proceed further, let us show now that the energy in any wavefunction is nonnegative:

$$\langle \psi | H | \psi \rangle = \int dx \left( \frac{\hbar^2}{2m} \left| \frac{d\psi}{dx} \right|^2 + \frac{1}{2} K x^2 |\psi|^2 \right) \ge 0.$$

Let us furthermore denote the state with lowest energy (ground state) as  $|0\rangle$  and its energy as  $E_0$ ,  $H|0\rangle = E_0|0\rangle$ . We claim that

$$a|0\rangle = 0. \tag{7}$$

In fact, if this was not true, then  $aH|0\rangle = E_0 a|0\rangle$  and making use of

$$[H,a] = -\hbar\omega a \tag{8}$$

we obtain that  $Ha|0\rangle = (E_0 - \hbar\omega)a|0\rangle$ , i.e. the energy of the state  $a|0\rangle$  is lower than  $E_0$ , in contradiction with our assumption that  $|0\rangle$  is the ground state. Thus Eq. 7 must hold.

Evaluating  $H|0\rangle$  making use of Eq. 7 we find that the energy of the ground state is  $E_0 = \hbar \omega/2$ . The wavefunction in x-respresentation satisfies the equation  $(\xi + d/d\xi)\psi = 0$ , from where  $\psi(\xi) \propto \exp(-\xi^2/2)$ .

Now let us consider the excited states of the oscillator. Let  $|n\rangle$  be such a state with energy  $E_n$ ,  $H|n\rangle = E_n|n\rangle$ . Then, making use of the commutator

$$[H, a^{\dagger}] = \hbar \omega a^{\dagger} \tag{9}$$

one finds readily that  $Ha^{\dagger}|n\rangle = (E_n + \hbar\omega)a^{\dagger}|n\rangle$ , i.e. the state  $a^{\dagger}|n\rangle$  is an eigenstate with an eigenvalue  $E_n + \hbar\omega$ .

EXERCISE Show by induction that the *n*-th normalized eigenvector (satisfying  $\langle n|n\rangle = 1$ ) and the corresponding eigenvalue are, respectively

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a^{\dagger}\right)^{n} |0\rangle,$$
  

$$E_{n} = \left(n + \frac{1}{2}\right) \hbar \omega.$$
(10)

Hint. Show first by induction

$$[a, (a^{\dagger})^{n}] = n (a^{\dagger})^{n-1}.$$

$$(11)$$

Making use of Eqs. 10,11 one finds readily that

$$\begin{aligned} a^{\dagger}|n\rangle &= \sqrt{n+1}|n+1\rangle, \\ a|n\rangle &= \sqrt{n}|n-1\rangle. \end{aligned}$$
 (12)

Eqs. 10,12 can be interpreted in the following way: the spectrum of the harmonic oscillator consists of states containing  $0,1,2,\ldots$  excitation quanta, each quantum being equal to  $\hbar\omega$ . The operator  $a^{\dagger}$  acting on a given state adds to it one quantum of energy and is therefore called a creation operator. The operator a removes one quantum of energy and is therefore called annihilation operator. From Eq. 12 it also follows that  $a^{\dagger}a|n\rangle = n|n\rangle$ , which means that the operator  $a^{\dagger}a$  measures the number of quanta. In what follows we talk interchangeably about particles and about the quanta.

The set of states  $\{|0\rangle, |1\rangle, |2\rangle, \ldots\}$  forms an orthonormal basis of the Hilbert space of the harmonic oscillator. Any physical operator acting in this Hilbert space should be expressible in terms of the coordinate and momentum operators, which read

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^{\dagger}),$$
  

$$p = i\sqrt{\frac{m\hbar\omega}{2}} (a^{\dagger} - a).$$
(13)

Since the action of a and  $a^{\dagger}$  is completely determined by Eqs. 12,7, also any matrix element of a physical operator can be calculated easily making use of Eq. 13.

The representation of physical operators Eq. 13 in terms of creation and annihilation operators and the interpretation Eq. 10 of the Hilbert space in terms of added quanta (or particles) is called second quantization in the literature.

### Schrödinger and Heisenberg pictures

So far we haven't talked about the time dependence of observables. In the Schrödinger picture we assume that the operators X of physical observables are independent of time, whereas the states  $|\psi\rangle$  are subject to time evolution governed by the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle. \tag{14}$$

As a result, the expectation value  $\langle X \rangle$  of the observable X becomes time dependent,  $\langle X \rangle(t) = \langle \psi(t) | X | \psi(t) \rangle$ . For a time independent Hamiltonian the time evolution of  $|\psi\rangle$  can be formally solved,

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$$

and therefore the time dependence of the expectation value can equivalently be written as

$$\langle X \rangle(t) = \langle \psi(0) | e^{iHt/\hbar} X e^{-iHt/\hbar} | \psi(0) \rangle = \langle \psi_H | X_H(t) | \psi_H \rangle, \tag{15}$$

where in the last equation we have defined the operators and states in the so-called Heisenberg picture:  $X_H(t) = e^{iHt/\hbar} X e^{-iHt/\hbar}$  and  $|\psi_H\rangle = |\psi(0)\rangle$ . The Heisenberg picture Eq. 15 thus offers an alternative view of the time evolution of expectation values: the states do not evolve with time, but the operators do. By taking the time derivative of the expression for  $X_H(t)$  we find

$$\frac{d}{dt}X_H = \frac{i}{\hbar}[H, X_H] + \left(\frac{\partial X}{\partial t}\right)_H,\tag{16}$$

where the second term on the right-hand side vanishes for an operator which is not explicitly time dependent (in the Schrödinger picture). Eq. 16 is called the equation of motion for the operator X. Making use of  $[H, X_H] = [H, X]_H$  and of Eqs. 9,8 in the equations of motion for the creation and annihilation operators of a harmonic oscillator, one finds readily that  $a_H^{\dagger}(t) = a^{\dagger}e^{i\omega t}$  and  $a_H(t) = ae^{-i\omega t}$ .

## Coherent states

Eigenstates of the annihilation operator are called coherent states which are useful in more advanced many body techniques. In what follows we show that the state

$$|z\rangle = e^{-|z|^2/2} e^{za^{\dagger}} |0\rangle,$$

where z is a complex number, is a coherent state. Here the function  $e^{za^{\dagger}}$  of a creation operator should be understood in terms of its Taylor expansion,  $e^{za^{\dagger}} = \sum_{n=0}^{\infty} (z^n/n!) (a^{\dagger})^n$ .

# EXERCISES

1. If  $f(a^{\dagger})$  is a function of the creation operator, show that

$$[a, f(a^{\dagger})] = \frac{df}{da^{\dagger}}.$$
(17)

Hint. Write down the (formal) Taylor expansion of  $f(a^{\dagger})$  and make use of Eq. 11.

2. Making use of Eq. 17 show that  $|z\rangle$  is a coherent state.

3. Show that the scalar product of two coherent states is

$$\langle u|z\rangle = e^{-(|u|^2 + |z|^2 - 2u^*z)/2}.$$

Thus the coherent states are not orthogonal to each other, but note that  $\langle z|z\rangle = 1$ . 4. Show that the system of coherent states is complete,

$$\int \frac{d^2 z}{\pi} |z\rangle \langle z| = 1.$$

5. Show that the time evolution of the expectation value of the coordinate and momentum is (with a real z)

$$\begin{aligned} \langle z|x(t)|z\rangle &= \sqrt{\frac{2\hbar}{m\omega}}z\cos\omega t, \\ \langle z|p(t)|z\rangle &= \sqrt{2\hbar m\omega}z\sin\omega t, \end{aligned}$$

i.e. they satisfy the classical equations of motion with amplitude proportional to z. 6. Show that the expectation value of energy

$$\langle z|H|z\rangle = \hbar\omega(|z|^2 + 1/2) = \frac{\langle p(t)\rangle^2}{2m} + \frac{1}{2}K\langle x(t)\rangle^2 + \hbar\omega/2,$$

i.e. it is given by its classical value, up to a shift equal to the ground state energy.

# LECTURE 2: SECOND QUANTIZATION - 'REAL' PARTICLES

In the previous lecture we have seen that excited states of an oscillator can be thought of as particles. In case of electromagnetic oscillations (photons) or lattice oscillations (phonons) these are very real particles which can be observed by numerous experimental means. Yet, at least in condensed matter physics, electrons, protons, and neutrons are in a sense more real, since their numbers we take as conserved, whereas photons and phonons can be created or annihilated, e.g. when an electron falls down from an excited state of an atom to its ground state. In this lecture we will concentrate on systems of many 'real' particles.

Consider first that in the system of interest there is only one particle. (For definiteness, we can think of a particle in a box  $L \times L \times L$  with periodic boundary conditions,  $\varphi(x + L, y, z) = \varphi(x, y, z)$  and similarly in the y and z directions.) All possible states of this particle form a Hilbert space. Let  $\{|a\rangle, |b\rangle, \ldots\}$  be an orthonormal basis of this Hilbert space. In the x-representation, the corresponding wavefunctions are  $\varphi_a(\mathbf{x}), \varphi_b(\mathbf{x}), \ldots$ 

For a system with only one particle it is irrelevant, whether the particle is a boson or a fermion. Now consider that we have many identical particles in the system. In Lecture 1 we have seen that the cases of fermions and bosons should be treated separately. We have chosen to start with bosons.

## Bosons

Consider first a system with two bosons in two different states  $|a\rangle$  and  $|b\rangle$ . Then it is easy to see that the normalised two-boson wavefunction (which must be symmetric under exchange of the coordinates 1 and 2 of the first and second particle) reads

$$\psi_{1,1,0,\dots}(1,2) = \frac{1}{\sqrt{2}} \left[ \varphi_a(1)\varphi_b(2) + \varphi_b(1)\varphi_a(2) \right],$$

where the index 1, 1, 0, ... denotes that states  $|a\rangle$  and  $|b\rangle$  are populated with one particle each, whereas all other one-particle states are empty. Now consider a general system of N bosons with  $N_1$  particles in the state  $|a\rangle$ ,  $N_2$  particles in the state  $|b\rangle$ , etc. Then the N-boson wavefunction which is symmetric under exchange of any two particles reads

$$\psi_{N_1,N_2,\dots}(1,2,\dots,N) = \sqrt{\frac{N_1!N_2!\dots}{N!}} \sum_{\{P\}} \varphi_{P_1}(1)\varphi_{P_2}(2)\dots\varphi_{P_N}(N),$$
(18)

where  $P_1, P_2, \ldots, P_N$  is a permutation of  $N_1$  indices  $a, N_2$  indices b, etc. The sum is to be taken over all different permutations. It is obvious that, once the basis of single-particle states is fixed, the many-body states are completely determined by specifying the numbers of particles occupying the single-particle states. Therefore instead of the wavefunction  $\psi_{N_1,N_2,\ldots}(1,2,\ldots,N)$  in **x**-representation we can talk about the state  $|N_1,N_2,\ldots\rangle$ . Let us show now that Eq. 18 is a normalised wavefunction:

$$\langle N_1, N_2, \dots | N_1, N_2, \dots \rangle = \frac{N_1! N_2! \dots}{N!} \sum_{\{P, P'\}} \int d1 \varphi_{P_1}^*(1) \varphi_{P_1}(1) \dots \int dN \varphi_{P_N}^*(N) \varphi_{P_N}(N)$$

$$= \frac{N_1!N_2!\dots}{N!} \sum_{\{P,P'\}} \delta_{P_1,P'_1}\dots\delta_{P_N,P'_N} = 1,$$

since the number of permutations is  $N!/N_1!N_2!\dots$ 

Any N-boson state can be written as a linear superposition of states of the type Eq. 18 which are seen to form a complete orthonormal basis of the Hilbert space of N-particle states.

From Eq. 18 one can see that the formula for the many-body wavefunction in **x**-representation representation is quite cumbersome, although the physical content is simple: the wavefunction contains  $N_1$  particles in state  $|a\rangle$ ,  $N_2$  particles in state  $|b\rangle$ , etc. In what follows we introduce an equivalent and simpler language for the description of many boson states:

- Let  $|0\rangle$  be the vacuum state, i.e. a state without particles.
- Let  $a_i$  and  $a_i^{\dagger}$  be creation and annihilation operators for the single-particle state *i* which satisfy the following (canonical) boson commutation relations:

$$[a_i, a_j^{\dagger}] = \delta_{ij},$$
  
$$[a_i, a_j] = [a_i^{\dagger}, a_j^{\dagger}] = 0.$$
 (19)

• Since the vacuum state contains no particles, we require that  $a_i|0\rangle = 0$  for all single-particle states *i*.

Making use of the techniques introduced in Lecture 1, one finds readily that

$$|N_1, N_2, \ldots\rangle = \frac{1}{\sqrt{N_1! N_2! \ldots}} \left(a_a^{\dagger}\right)^{N_1} \left(a_b^{\dagger}\right)^{N_2} \ldots |0\rangle$$

is a normalized N-particle state describing the same physics as Eq. 18.

## Fermions

Let us consider now systems of many fermions. For two particles in one-particle states  $|a\rangle$  and  $|b\rangle$ , the wavefunction can be written

$$\psi_{a,b}(1,2) = \frac{1}{\sqrt{2}} \left[\varphi_a(1)\varphi_b(2) - \varphi_b(1)\varphi_a(2)\right],$$

with notations similar as in the boson case. Note that, unlike in the boson case, if the states  $|a\rangle$  and  $|b\rangle$  are equal, the wavefunction vanishes. This implies the famous Pauli principle that two fermions can't occupy the same quantum state. It should be stressed at this point that the symbol 1 for the coordinates of the first particle should be understood as a shorthand for both the spatial and the spin coordinate,  $1 = (\mathbf{x}_1, \sigma_1)$  (and similarly for other particles).

In other words, the Pauli principle implies that the sequence of occupation numbers  $N_1, N_2, \ldots$  (where the ordering of the one-particle states is fixed once forever) may contain only the numbers 0 and 1. One verifies easily that the general N-particle wavefunction which is antisymmetric under exchange of any two coordinates reads

$$\psi_{a_1,a_2,\dots,a_N}(1,2,\dots,N) = \frac{1}{\sqrt{N!}} \sum_{\{P\}} (-1)^P \varphi_{P_1}(1) \varphi_{P_2}(2) \dots \varphi_{P_N}(N),$$
(20)

where  $\psi_{a_1,a_2,\ldots,a_N}$  means that only the one-particle states  $|a_1\rangle, |a_2\rangle, \ldots, |a_N\rangle$  are occupied and the remaining states are empty.  $P_1, P_2, \ldots, P_N$  is a permutation of the states  $|a_1\rangle, |a_2\rangle, \ldots, |a_N\rangle$ , and the factor  $(-1)^P$  equals 1 and -1 for those permutations, which can be arrived at after even and odd numbers of pair exchanges, respectively.

EXERCISE Show that the wavefunction Eq. 20 is normalized.

In what follows we adapt the method of second quantization to the case of fermions. We start with the following definitions:

- Let  $|0\rangle$  be the vacuum state, i.e. a state without particles.
- Let  $c_i$  and  $c_i^{\dagger}$  be creation and annihilation operators for the single-particle state *i* which satisfy the following (canonical) fermion anticommutation relations:

$$\{c_i, c_j^{\dagger}\} = \delta_{ij},$$
  
$$\{c_i, c_j\} = \{c_i^{\dagger}, c_j^{\dagger}\} = 0.$$
 (21)

(The anticommutator is defined as  $\{X, Y\} = XY + YX$ .)

• Since the vacuum state contains no particles, we require that  $c_i|0\rangle = 0$  for all singleparticle states *i*.

In what follows we will show that the basis states of the N-fermion Hilbert space, Eq. 20, can be written in the following second-quantized form

$$|\psi_{a_1,a_2,\ldots,a_N}\rangle = c_{a_1}^{\dagger}c_{a_2}^{\dagger}\ldots c_{a_N}^{\dagger}|0\rangle.$$

In fact, N-particle states in which the fermions occupy different sets  $\{a_1, a_2, \ldots, a_N\}$  and  $\{b_1, b_2, \ldots, b_N\}$  of single-particle states are orthogonal to each other. To see this, let us assume that the state b is contained in the set  $\{b_1, b_2, \ldots, b_N\}$  but not in  $\{a_1, a_2, \ldots, a_N\}$ . We find

$$\langle \psi_{b_1, b_2, \dots, b_N} | \psi_{a_1, a_2, \dots, a_N} \rangle = \langle 0 | c_{b_N} \dots c_{b_2} c_{b_1} c_{a_1}^{\dagger} c_{a_2}^{\dagger} \dots c_{a_N}^{\dagger} | 0 \rangle = 0,$$

since the annihilation operator  $c_b$  can be moved to the right so that it is the rightmost one of the 2N creation and annihilation operators (with possibly changing the sign of the overlap), but  $c_b|0\rangle = 0$ . On the other hand, we find

$$\langle \psi_{a_1,a_2,\dots,a_N} | \psi_{a_1,a_2,\dots,a_N} \rangle = \langle 0 | c_{a_N} \dots c_{a_2} c_{a_1} c_{a_1}^{\dagger} c_{a_2}^{\dagger} \dots c_{a_N}^{\dagger} | 0 \rangle$$

$$= \langle 0 | c_{a_N} \dots c_{a_2} (1 - c_{a_1}^{\dagger} c_{a_1}) c_{a_2}^{\dagger} \dots c_{a_N}^{\dagger} | 0 \rangle$$

$$= \langle 0 | c_{a_N} \dots c_{a_2} c_{a_2}^{\dagger} \dots c_{a_N}^{\dagger} | 0 \rangle$$

$$= \dots$$

$$= \langle 0 | 0 \rangle = 1,$$

i.e. the state  $|\psi_{a_1,a_2,\ldots,a_N}\rangle$  is normalized. We have used that  $[c_{a_1}^{\dagger}c_{a_1}, c_{a_j}^{\dagger}] = 0$  for  $j \neq 1$ . Note that all states  $a_1, a_2, \ldots, a_N$  must be different, otherwise  $|\psi_{a_1,a_2,\ldots,a_N}\rangle = 0$  (since from the anticommutation relations it follows  $c_a^{\dagger}c_a^{\dagger} = 0$ ), i.e. the Pauli principle is satisfied. Finally, let us note that if the set  $\{b_1, b_2, \ldots, b_N\}$  is a permutation of  $\{a_1, a_2, \ldots, a_N\}$ , then

$$\langle \psi_{b_1,b_2,\dots,b_N} | \psi_{a_1,a_2,\dots,a_N} \rangle = \pm 1,$$

the plus (minus) sign obtaining for an even (odd) permutation. Thus, the order of operators is not irrelevant as in the case of bosons.

EXERCISE Show that  $c_a^{\dagger}c_a|\psi_{a_1,a_2,\ldots,a_N}\rangle = n_a|\psi_{a_1,a_2,\ldots,a_N}\rangle$ , where  $n_a = 1$  if the state *a* is among the states  $a_1, a_2, \ldots, a_N$  and  $n_a = 0$  otherwise. Thus the operator  $c_a^{\dagger}c_a$  measures the number of particles in the single-particle state *a*.

### One-particle operators

Having defined the many-particle states in the language of second quantization, let us discuss now how to express the operators in terms of creation and annihilation operators. Let us start with the so-called one-particle operators F, which can be written as

$$F = \sum_{i=1}^{N} f_i,$$

where the sum runs over all particles in the system and  $f_i$  is an operator acting on the *i*-th particle. The kinetic energy, total momentum, *z*-component of the total spin, etc. are examples of such operators.

Let us consider that basis of one-particle states  $|a\rangle, |b\rangle, \ldots$  which diagonalizes the oneparticle operators f,  $\langle a|f|b\rangle = f_a \delta_{ab}$ . It is obvious that in this basis the total quantity F can be calculated by summing over all states and counting how many particles occupy them,

$$F = \sum_{a} f_{a} c_{a}^{\dagger} c_{a} = \sum_{ab} \langle a | f | b \rangle c_{a}^{\dagger} c_{b}$$

where for definiteness we have assumed the fermion case, but the boson case has the same form. The second equation, although at first sight unnecessarily complicated, will be used later.

Finally, let us change the basis set of one-particle states to  $|\alpha\rangle = \sum_{a} U_{\alpha a} |a\rangle$  (the old basis states are denoted by latin and the new ones by greek letters). The hermitian conjugate equation reads  $\langle \alpha | = \sum_{a} U_{\alpha a}^* \langle a |$  and therefore

$$\delta_{\alpha\beta} = \langle \alpha | \beta \rangle = \sum_{ab} U^*_{\alpha a} U_{\beta b} \langle a | b \rangle = \sum_{a} U^*_{\alpha a} U_{\beta a} = \sum_{a} U_{\beta a} \left( U^{\dagger} \right)_{a\alpha} = \left( U U^{\dagger} \right)_{\beta\alpha}$$

Thus a transformation between orthonormal bases needs to be unitary,  $UU^{\dagger} = 1$  or  $U^{\dagger} = U^{-1}$ . From here it follows that  $U^{\dagger}U = 1$  or  $\sum_{a} U^*_{a\alpha} U_{a\beta} = \delta_{\alpha\beta}$ . The inverse transformation from the new basis to the old one therefore reads

$$\sum_{\alpha} U_{\alpha a}^* |\alpha\rangle = \sum_{\alpha b} U_{\alpha a}^* U_{\alpha b} |b\rangle = \sum_{b} \delta_{ab} |b\rangle = |a\rangle.$$

Since the wavefunctions can be thought of as a result of the action of creation operators on the vacuum, we have the following transformation rules

$$c_{a}^{\dagger} = \sum_{\alpha} U_{\alpha a}^{*} c_{\alpha}^{\dagger},$$

$$c_{a} = \sum_{\alpha} U_{\alpha a} c_{\alpha}.$$
(22)

Inserting Eq. 22 into the expression for F we find

$$F = \sum_{ab} \langle a|f|b\rangle c_a^{\dagger} c_b = \sum_{ab} \sum_{\alpha\beta} U_{\alpha a}^* \langle a|f|b\rangle U_{\beta b} c_{\alpha}^{\dagger} c_{\beta} = \sum_{\alpha\beta} \langle \alpha|f|\beta\rangle c_{\alpha}^{\dagger} c_{\beta},$$
(23)

which is the general expression for one body operators, valid both for bosons and fermions.

### EXERCISES

1. Consider electrons (fermions with spin 1/2) whose complete one-particle basis set consists of states  $|\alpha \uparrow\rangle$  and  $|\alpha \downarrow\rangle$ , where  $|\alpha\rangle$  is a complete set of orbital states and  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are the two possible projections of the electron spin on a fixed chosen spin quantization axis. Let us define the operators

$$S^{+} = \sum_{\alpha} c^{\dagger}_{\alpha\uparrow} c_{\alpha\downarrow},$$
  

$$S^{-} = \sum_{\alpha} c^{\dagger}_{\alpha\downarrow} c_{\alpha\uparrow}.$$
(24)

a) Compute  $S^z$  from the expression  $S^z = [S^+, S^-]/2$ .

b) Show that  $[S^z, S^+] = S^+$  and  $[S^z, S^-] = -S^-$ .

c) What is the physical meaning of the operators  $S^x = (S^+ + S^-)/2$ ,  $S^y = (S^+ - S^-)/2i$ , and  $S^z$ ?

2. Let us define the operator  $\mathbf{S}^2 = (S^x)^2 + (S^y)^2 + (S^z)^2$  and let us denote its eigenvalues as S(S+1). Show that the following two-electron states are eigenstates of  $\mathbf{S}^2$  and  $S^z$ . Compute the eigenvalues S and  $S^z$  for these states.

$$\begin{split} |\psi\rangle &= \frac{1}{\sqrt{2}} (c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\beta\downarrow} - c^{\dagger}_{\alpha\downarrow} c^{\dagger}_{\beta\uparrow}) |0\rangle, \\ |\chi_1\rangle &= c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\beta\uparrow} |0\rangle, \\ |\chi_0\rangle &= \frac{1}{\sqrt{2}} (c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\beta\downarrow} + c^{\dagger}_{\alpha\downarrow} c^{\dagger}_{\beta\uparrow}) |0\rangle, \\ |\chi_{-1}\rangle &= c^{\dagger}_{\alpha\downarrow} c^{\dagger}_{\beta\downarrow} |0\rangle. \end{split}$$

3. Show that the states from exercise 2 form a complete orthonormal basis in the Hilbert space of two-electron states built from two orbitals  $|\alpha\rangle$  and  $|\beta\rangle$ .

# LECTURE 3: TWO-ELECTRON SYSTEMS

# Two body operators

In what follows we seek an expression for a general two-body operator

$$G = \frac{1}{2} \sum_{i \neq j} g_{ij},$$

where the sum is over all pairs of particles (we exclude the interaction of a particle with itself) and  $g_{ij}$  is an operator acting on particles *i* and *j*. The most commonly met example

of a two-body operator is the interaction energy of a system with two-body interactions, e.g. the Coulomb energy of charged particles. We will frequently make use of the matrix element

$$\langle ab|g|cd\rangle = \int di \int dj \,\varphi_a^*(i)\varphi_b^*(j)g_{ij}\varphi_c(i)\varphi_d(j).$$
<sup>(25)</sup>

Note that  $\langle ab|g|cd \rangle^* = \langle cd|g|ab \rangle$ . Moreover, for even operators  $g_{ij} = g_{ji}$ , we also have  $\langle ab|g|cd \rangle = \langle ba|g|dc \rangle$ . These two properties imply that the matrix elements  $\langle ab|g|ab \rangle$  and  $\langle ab|g|ba \rangle$  are both real.

Let us consider that basis of single-particle states which diagonalizes the interaction function g,  $\langle ab|g|cd \rangle = \delta_{ac}\delta_{bd}\langle ab|g|ab \rangle$ . In this case also the two-body operator G remains diagonal in the basis Eq. 20 of the N-fermion Hilbert space (or, for N-boson states, in the basis Eq. 18). Therefore the operator G can be expressed as

$$G = \frac{1}{2} \sum_{ab} \langle ab | g | ab \rangle P_{ab},$$

where  $P_{ab}$  is an operator counting the number of particle pairs. If  $|a\rangle \neq |b\rangle$  then  $P_{ab} = n_a n_b$ (where  $n_a$  is the operator of the number of particles), whereas for  $|a\rangle = |b\rangle$  we have  $P_{aa} = n_a(n_a - 1)$ . Combining the two cases, we can write  $P_{ab} = n_a n_b - \delta_{ab} n_a$ . In terms of creation and annihilation operators we thus obtain  $P_{ab} = c_a^{\dagger} c_a c_b^{\dagger} c_b - \delta_{ab} c_a^{\dagger} c_a$  and therefore in our one-particle basis we can write

$$G = \frac{1}{2} \sum_{ab} \langle ab|g|ab \rangle (c_a^{\dagger} c_a c_b^{\dagger} c_b - \delta_{ab} c_a^{\dagger} c_a) = \frac{1}{2} \sum_{abcd} \langle ab|g|cd \rangle (c_a^{\dagger} c_c c_b^{\dagger} c_d - \delta_{cb} c_a^{\dagger} c_d).$$

Now we observe that making use of canonical commutation (anticommutation) relations we can write  $c_a^{\dagger}c_c c_b^{\dagger}c_d - \delta_{cb}c_a^{\dagger}c_d = c_a^{\dagger}c_b^{\dagger}c_dc_c$ , an expression valid both for fermions and bosons. If we perform the transformation Eq. 22 to a general basis, making use of

$$\sum_{abcd} U^*_{\alpha a} U^*_{\beta b} U_{\delta d} U_{\gamma c} \langle ab | g | cd \rangle = \langle \alpha \beta | g | \gamma \delta \rangle$$

we find the final result for a two-particle operator (valid both for fermions and bosons)

$$G = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | g | \gamma\delta \rangle c^{\dagger}_{\alpha} c^{\dagger}_{\beta} c_{\delta} c_{\gamma}.$$
<sup>(26)</sup>

## Atom of carbon - Hund's rules

The total Hamiltonian of an atom can be written as  $H = H_0 + V$ , where  $H_0$  contains the kinetic energy of the electrons and the Coulomb interactions between the electrons and the nucleus. On the other hand, V describes the Coulomb repulsion between the electrons,  $V = 2^{-1} \sum_{i \neq j} v_{ij}$ . The energy levels of the  $H_0$  part of the Hamiltonian of a multielectron atom can be classified by the same quantum numbers as the hydrogen atom. The electronic configuration of the carbon atom is therefore  $1s^22s^22p^2$ . There are three p orbitals, whose angular dependence is

$$p_1(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi},$$

$$p_0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta,$$
$$p_{-1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}$$

This means that the 2p shell is only partially filled. There are 6!/(2!(6-2)!) = 15 ways in which the two electrons can be distributed among 6 available one-particle states (3 orbital states  $\times$  2 spin states). In other words, one can construct 15 states of the type  $c^{\dagger}_{a\sigma}c^{\dagger}_{b\sigma'}|0\rangle$ , where a, b are arbital indices and  $\sigma, \sigma'$  are spin indices.

We ask the question which of these 15 two-particle states minimizes the total energy of the atom. In order to answer this question, in what follows we calculate the first order correction to energy with respect to the perturbation V. If we attempt to solve this question by brute force, we need to diagonalize a matrix  $15 \times 15$ . In search of an analytical solution, we look for symmetries of the problem which help us to reduce the dimensionality of the problem. To this end let us define the following set of operators

$$L^{z} = \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{1\sigma} - c_{-1\sigma}^{\dagger} c_{-1\sigma}),$$
  

$$L^{+} = \sqrt{2} \sum_{\sigma} (c_{0\sigma}^{\dagger} c_{-1\sigma} + c_{1\sigma}^{\dagger} c_{0\sigma}),$$
  

$$L^{-} = \sqrt{2} \sum_{\sigma} (c_{-1\sigma}^{\dagger} c_{0\sigma} + c_{0\sigma}^{\dagger} c_{1\sigma}).$$
(27)

### EXERCISES

1. Show that  $[L^+, L^-] = L^z$  and  $[L^z, L^{\pm}] = \pm L^{\pm}$ . This means that  $\mathbf{L} = (L^x, L^y, L^z)$ (where  $L^x = (L^+ + L^-)/2$  and  $L^y = (L^+ - L^-)/2i$ ) is the operator of orbital momentum. 2. Show that  $[L^i, S^j] = 0$ , where the spin operator **S** has been defined in Eq. 24.

Since the Hamiltonian V is independent of spin and rotationally invariant, we must have  $[V, L^i] = [V, S^i] = 0$ . This means that the eigenstates of V can be chosen so as to simultaneously diagonalize the commuting set of operators  $\mathbf{L}^2, L^z, \mathbf{S}^2, L^z$ .

Let us start by constructing the state L = 2,  $L^z = 2$ . There is only 1 such state, in which both electrons are placed in the same orbital  $|p_1\rangle$ . By subsequent application of the lowering operator  $L^-$  to this state we obtain the following 5 states:

$$\begin{aligned} |D_{2}\rangle &= c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}|0\rangle, \\ |D_{1}\rangle &= 2^{-1/2}(c_{1\uparrow}^{\dagger}c_{0\downarrow}^{\dagger} + c_{0\uparrow}^{\dagger}c_{1\downarrow}^{\dagger})|0\rangle, \\ |D_{0}\rangle &= 6^{-1/2}(c_{1\uparrow}^{\dagger}c_{-1\downarrow}^{\dagger} + 2c_{0\uparrow}^{\dagger}c_{0\downarrow}^{\dagger} + c_{-1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger})|0\rangle, \\ D_{-1}\rangle &= 2^{-1/2}(c_{0\uparrow}^{\dagger}c_{-1\downarrow}^{\dagger} + c_{-1\uparrow}^{\dagger}c_{0\downarrow}^{\dagger})|0\rangle, \\ D_{-2}\rangle &= c_{-1\uparrow}^{\dagger}c_{-1\downarrow}^{\dagger}|0\rangle. \end{aligned}$$
(28)

One can show easily that  $\mathbf{S}^2 | D_2 \rangle = 0$ . Since  $\mathbf{S}^2$  commutes with  $L^-$ , all states  $|D_i\rangle$  have S = 0 (they are spin singlets). On the other hand, by construction we have  $L^z | D_i \rangle = i | D_i \rangle$  and  $\mathbf{L}^2 | D_i \rangle = L(L+1) | D_i \rangle$  with L = 2.

Next we construct all states with S = 1 and  $S^z = 1$ . This requires that both electrons have spin up and there are three such states:

$$|P_{11}\rangle = c_{1\uparrow}^{\dagger}c_{0\uparrow}^{\dagger}|0\rangle,$$

$$|P_{01}\rangle = c^{\dagger}_{1\uparrow}c^{\dagger}_{-1\uparrow}|0\rangle, |P_{-11}\rangle = c^{\dagger}_{0\uparrow}c^{\dagger}_{-1\uparrow}|0\rangle.$$
(29)

The notation in Eq. 29 is chosen so that the first index n in  $|P_{nm}\rangle$  measures  $L^z$ ,  $L^z|P_{nm}\rangle = n|P_{nm}\rangle$ , whereas the second index measures  $S^z$ ,  $S^z|P_{nm}\rangle = m|P_{nm}\rangle$ . By subsequent application of the spin lowering operator  $S^-$  to each of the three states Eq. 29, we obtain in total 9 states of the type  $|P_{nm}\rangle$ , where n = -1, 0, 1 and m = -1, 0, 1. Moreover, one can easily show that all  $|P_{nm}\rangle$  states have L = 1 and S = 1.

So far, we have constructed 5 states  $|D_i\rangle$  and 9 states  $|P_{nm}\rangle$ . In order to proceed, we need to find the last linearly independent combination of the states  $c^{\dagger}_{a\sigma}c^{\dagger}_{b\sigma'}|0\rangle$ . In order to find it, let us note that there exist 3 combinations of a, b and  $\sigma, \sigma'$  which lead to  $S^z = L^z = 0$ , namely  $c^{\dagger}_{1\uparrow}c^{\dagger}_{-1\downarrow}|0\rangle$ ,  $c^{\dagger}_{0\uparrow}c^{\dagger}_{0\downarrow}|0\rangle$ , and  $c^{\dagger}_{-1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle$ . On the other hand, so far we have constructed only 2 states with  $S^z = L^z = 0$ , namely  $|D_0\rangle$  and  $|P_{00}\rangle =$  $2^{-1/2}(c^{\dagger}_{1\uparrow}c^{\dagger}_{-1\downarrow} + c^{\dagger}_{1\downarrow}c^{\dagger}_{-1\uparrow})|0\rangle$ . The remaining linearly independent state with  $S^z = L^z = 0$ is easily found to be

$$|S\rangle = 3^{-1/2} (c_{1\uparrow}^{\dagger} c_{-1\downarrow}^{\dagger} - c_{0\uparrow}^{\dagger} c_{0\downarrow}^{\dagger} + c_{-1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger})|0\rangle = \sqrt{\frac{2}{3}} |\alpha\rangle - \sqrt{\frac{1}{3}} c_{0\uparrow}^{\dagger} c_{0\downarrow}^{\dagger}|0\rangle, \tag{30}$$

where  $|\alpha\rangle = 2^{-1/2} (c_{1\uparrow}^{\dagger} c_{-1\downarrow}^{\dagger} - c_{1\downarrow}^{\dagger} c_{-1\uparrow}^{\dagger}) |0\rangle$ . One finds easily that the  $|S\rangle$  state is chacterized by L = S = 0.

Summarizing, a basis of the (15 dimensional) Hilbert space can be found, in which every basis vector has different quantum numbers  $L, L^z, S, S^z$ . Therefore the Hamiltonian V in this basis is diagonal. Moreover, since the energy should not depend on the directions of the spin and orbital momenta, one of the levels (corresponding to the  $|S\rangle$  state) will be nondegenerate, one five-fold degenerate (the  $|D_i\rangle$  states), and one nine-fold degenerate (the  $|P_{nm}\rangle$  states). Therefore it is sufficient to calculate three matrix elements in order to determine the full spectrum of the problem.

EXERCISE Show that

$$\begin{split} E(S) &= \langle S|V|S \rangle = \frac{2}{3} \langle \alpha | v | \alpha \rangle + \frac{1}{3} \langle 00|v|00 \rangle - \frac{2}{3} \left( \langle 00|v|1-1 \rangle + \langle 00|v|-11 \rangle \right), \\ E(P) &= \langle P_{11}|V|P_{11} \rangle = \langle 10|v|10 \rangle - \langle 10|v|01 \rangle, \\ E(D) &= \langle D_2|V|D_2 \rangle = \langle 11|v|11 \rangle, \end{split}$$

where  $\langle \alpha | v | \alpha \rangle = \langle 1 - 1 | v | 1 - 1 \rangle + \langle 1 - 1 | v | - 11 \rangle$ .

Making use of the techniques of atomic physics, one can show

$$\begin{array}{rcl} \langle 00|v|00\rangle &=& \langle 11|v|11\rangle + \langle 10|v|01\rangle, \\ \langle 10|v|10\rangle &=& \langle 11|v|11\rangle - \langle 10|v|01\rangle, \\ \langle 1-1|v|-11\rangle &=& 2\langle 10|v|01\rangle, \\ \langle 1-1|v|1-1\rangle &=& \langle 11|v|11\rangle, \\ \langle 00|v|1-1\rangle &=& \langle 00|v|-11\rangle = -\langle 10|v|01\rangle. \end{array}$$

This enables us to express the energies E(S), E(P), and E(D) in terms of only two matrix elements,  $\langle 11|v|11 \rangle$  and  $\langle 10|v|01 \rangle$ ,

$$E(S) = \langle 11|v|11\rangle + 3\langle 10|v|01\rangle,$$

$$E(D) = \langle 11|v|11\rangle, E(P) = \langle 11|v|11\rangle - 2\langle 10|v|01\rangle.$$
(31)

For repulsive interactions which decay with increasing distance between the particles (like Coulomb interactions) we expect  $\langle ab|v|ba\rangle > 0$ . This can be shown explicitly for contact interactions, where  $v(\mathbf{x} - \mathbf{y}) = V\delta(\mathbf{x} - \mathbf{y})$ :

$$\langle ab|v|ba\rangle = \int d^3\mathbf{x} \int d^3\mathbf{y} \varphi_a^*(\mathbf{x}) \varphi_b^*(\mathbf{y}) v(\mathbf{x} - \mathbf{y}) \varphi_b(\mathbf{x}) \varphi_a(\mathbf{y}) = V \int d^3\mathbf{x} |\varphi_a(\mathbf{x})|^2 |\varphi_b(\mathbf{x})|^2 \ge 0.$$

This then means that Eq. 31 is completely consistent with Hund's rules:

- The ground state of an atom with an incomplete shell has the maximal total spin. (In our case the states  $|P_{ij}\rangle$  with S = 1.)
- Within the subspace with a given total spin, energy is minimized by the state with the maximal orbital momentum. (In our case, within the subspace with S = 0, the states  $|D_i\rangle$  with L = 2 have lower energy than the state  $|S\rangle$  with L = 0.)

The reason why spin is maximized in the ground state is the following. When two electrons have a parallel spin, due to Pauli's principle they try to avoid being close to each other. This lowers their Coulomb interaction energy.

## Hydrogen molecule

As another example of a two-electron system, let us consider now the hydrogen molecule. Within the simplest model, we can restrict the Hilbert space of one-particle states to two orthogonal orbitals, one of them centered at the atom 1 and an identical one centered around the atom 2. We consider the following model of the hydrogen molecule

$$H = -t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}), \qquad (32)$$

where the first term describes hopping of electrons between states  $|1\rangle$  and  $|2\rangle$  (parametrized by the hopping amplitude t) and the second term (in which  $n_{a\sigma} = c^{\dagger}_{a\sigma}c_{a\sigma}$ ) originates in the Coulomb repulsion between the electrons. Note that the full Coulomb interaction  $V(\mathbf{x} - \mathbf{y})$  would include also other matrix elements Eq. 25 besides

$$U = \int d^3 \mathbf{x} \int d^3 \mathbf{y} |\varphi_1(\mathbf{x})|^2 |\varphi_1(\mathbf{y})|^2 V(\mathbf{x} - \mathbf{y}) = \int d^3 \mathbf{x} \int d^3 \mathbf{y} |\varphi_2(\mathbf{x})|^2 |\varphi_2(\mathbf{y})|^2 V(\mathbf{x} - \mathbf{y}),$$

but all of them are neglected in the so-called Hubbard model Eq. 32, because they are much smaller.

There are two electrons in the hydrogen molecule. The Hilbert space of two-particle states consists of 4!/(2!(4-2)!) = 6 states of the type  $c^{\dagger}_{a\sigma}c^{\dagger}_{b\sigma'}|0\rangle$ . Thus, in order to find the ground state of the hydrogen molecule, we need to diagonalize the Hamiltonian matrix  $6 \times 6$ . Making use of the symmetries of the problem, this task can be performed completely.

EXERCISE Show that the Hamiltonian Eq. 32 commutes with the total spin operator,  $[H, \mathbf{S}^2] = [H, S^z] = 0.$ 

Next we define a parity operator P. Its physical meaning is to interchange sites 1 and 2. Therefore we require  $P^2 = 1$ ,  $Pc_{1\sigma}^{\dagger}P = c_{2\sigma}^{\dagger}$ , and  $Pc_{1\sigma}P = c_{2\sigma}$ . The vacuum state does not change under interchange of 1 and 2, i.e.  $P|0\rangle = |0\rangle$ . One verifies easily that [H, P] = 0 and  $[P, \mathbf{S}^2] = [P, S^z] = 0$ .

Now we construct linear combinations of the basis states  $c_{a\sigma}^{\dagger} c_{b\sigma'}^{\dagger} |0\rangle$  which are simultaneous eigenstates of P,  $\mathbf{S}^2$ , and  $S^z$ . We start with the state S = 1,  $S^z = 1$  and apply the spin lowering operator  $S^-$  to it:

$$\begin{aligned} |T_1\rangle &= c_{1\uparrow}^{\dagger}c_{2\uparrow}^{\dagger}|0\rangle, \\ |T_0\rangle &= 2^{-1/2}(c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger} + c_{1\downarrow}^{\dagger}c_{2\uparrow}^{\dagger})|0\rangle, \\ |T_{-1}\rangle &= c_{1\downarrow}^{\dagger}c_{2\downarrow}^{\dagger}|0\rangle. \end{aligned}$$

One finds readily that the parity of these so-called triplet states is P = -1. On the other hand, the state orthogonal to  $|T_0\rangle$ ,

$$|S_1\rangle = 2^{-1/2} (c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} - c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger})|0\rangle,$$

has quantum numbers  $S = S^z = 0$  and P = 1. The two remaining states involve doubly occupied orbitals 1 and 2:

$$|S_2\rangle = 2^{-1/2} (c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} + c_{2\uparrow}^{\dagger} c_{2\uparrow}^{\dagger})|0\rangle$$

has quantum numbers  $S = S^z = 0$  and P = 1, whereas

$$|S_3\rangle = 2^{-1/2} (c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} - c_{2\uparrow}^{\dagger} c_{2\uparrow}^{\dagger}) |0\rangle$$

is characterized by  $S = S^z = 0$  and P = -1.

Note that all of the above states, except for the pair of states  $|S_1\rangle$  and  $|S_2\rangle$ , have different quantum numbers and therefore all off-diagonal matrix elements of H in this new basis vanish, except for  $\langle S_1|H|S_2\rangle$  and its hermitian conjugate.

EXERCISE Find the ground state (and the corresponding ground-state energy) of the hydrogen molecule described by the Hubbard model Eq. 32.

# The Hartree-Fock method

The hydrogen molecule example shows that the ground state of a many particle system is seldom a single Slater determinant (in this section we restrict our discussion to the fermion case). Nevertheless, usually a good first approximation to the ground state can be obtained, if we look for that Slater determinant, which minimizes the ground state energy within the subspace of Slater-determinant states. The crucial step is to find the corresponding set of single-particle states, out of which the Slater determinant is built. This method is called the Hartree-Fock method after its inventors.

Let us assume that the wavefunctions  $\varphi_{\alpha\sigma}(\mathbf{r})$  form the optimal single-particle basis we are looking for. Let furthermore  $|\Psi\rangle$  be the Slater determinant formed making use of  $\varphi_{\alpha\sigma}(\mathbf{r})$ . Then the expectation value of the interaction energy in the Hartree-Fock state  $|\Psi\rangle$  reads

$$\begin{split} \langle \Psi | H_{\text{int}} | \Psi \rangle &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \sum_{\sigma\sigma'} \langle \alpha\beta | V | \gamma\delta \rangle \langle \Psi | c^{\dagger}_{\alpha\sigma} c^{\dagger}_{\beta\sigma'} c_{\delta\sigma'} c_{\gamma\sigma} | \Psi \rangle \\ &= \frac{1}{2} \sum_{\alpha\beta} \sum_{\sigma\sigma'} \left( \langle \alpha\beta | V | \alpha\beta \rangle n_{\alpha\sigma} n_{\beta\sigma'} - \langle \alpha\beta | V | \beta\alpha \rangle n_{\alpha\sigma} n_{\beta\sigma'} \delta_{\sigma\sigma'} \right), \end{split}$$

since the same states which were annihilated by  $c_{\delta\sigma'}c_{\gamma\sigma}$  have to be restored back by  $c^{\dagger}_{\alpha\sigma}c^{\dagger}_{\beta\sigma'}$ . It is worth to emphasize that the operators  $c^{\dagger}_{\alpha\sigma}$  and  $c_{\alpha\sigma}$  create and annihilate the states  $\varphi_{\alpha\sigma}(\mathbf{r})$ . If we used another basis for the creation and annihilation operators, the result for  $\langle \Psi | H_{\text{int}} | \Psi \rangle$  would not be that simple. Making use of the definition of the matrix elements  $\langle \alpha\beta | V | \gamma\delta \rangle$  and adding the kinetic energy  $H_0$  we can write the total energy  $E[\Psi]$  of the state  $|\Psi\rangle$  as

$$\begin{split} E[\Psi] &= \sum_{\alpha\sigma} \int d^3 \mathbf{x} \varphi_{\alpha\sigma}^*(\mathbf{x}) H_0 \varphi_{\alpha\sigma}(\mathbf{x}) \\ &+ \frac{1}{2} \sum_{\alpha\beta\sigma\sigma'} \int d^3 \mathbf{x} \int d^3 \mathbf{y} \varphi_{\alpha\sigma}^*(\mathbf{x}) \varphi_{\beta\sigma'}^*(\mathbf{y}) V(\mathbf{x} - \mathbf{y}) \left[ \varphi_{\beta\sigma'}(\mathbf{y}) \varphi_{\alpha\sigma}(\mathbf{x}) - \delta_{\sigma\sigma'} \varphi_{\alpha\sigma}(\mathbf{y}) \varphi_{\beta\sigma'}(\mathbf{x}) \right], \end{split}$$

where the sums are to be taken over occupied states. Let us minimize now  $E[\Psi]$  with the boundary condition  $\int d^3 \mathbf{x} \varphi^*_{\alpha\sigma}(\mathbf{x}) \varphi_{\alpha\sigma}(\mathbf{x}) = 1$ , the latter being described by a Lagrange multiplier  $\varepsilon_{\alpha\sigma}$ . We obtain

$$H_{0}\varphi_{\alpha\sigma}(\mathbf{x}) + \sum_{\beta\sigma'} \int d^{3}\mathbf{y}\varphi_{\beta\sigma'}^{*}(\mathbf{y})V(\mathbf{x}-\mathbf{y})\left[\varphi_{\beta\sigma'}(\mathbf{y})\varphi_{\alpha\sigma}(\mathbf{x}) - \delta_{\sigma\sigma'}\varphi_{\alpha\sigma}(\mathbf{y})\varphi_{\beta\sigma'}(\mathbf{x})\right] = \varepsilon_{\alpha\sigma}\varphi_{\alpha\sigma}(\mathbf{x}),$$
(33)

which is the Hartree-Fock equation for the optimal one-electron orbitals. Note that if  $\beta \sigma' = \alpha \sigma$ , the interaction term vanishes. This means that a particle does not interact with itself. Eq. 33 can be written in the form of an ordinary Schrödinger equation  $H_{HF}\varphi_{\alpha\sigma}(\mathbf{x}) = \varepsilon_{\alpha\sigma}\varphi_{\alpha\sigma}(\mathbf{x})$ , where  $\varepsilon_{\alpha\sigma}$  can be interpreted as the Hartree-Fock energy of the single-particle state  $\varphi_{\alpha\sigma}(\mathbf{x})$ . The effective Hamiltonian  $H_{HF}$  acts on a wavefunction  $\varphi_{\sigma}(\mathbf{x})$  as follows:

$$H_{HF}\varphi_{\sigma}(\mathbf{x}) = [H_0 + V_H(\mathbf{x})]\varphi_{\sigma}(\mathbf{x}) - \int d^3 \mathbf{y} V_{\sigma}(\mathbf{x} - \mathbf{y})\varphi_{\sigma}(\mathbf{y}).$$

The potentials  $V_H(\mathbf{x})$  and  $V_{\sigma}(\mathbf{x} - \mathbf{y})$  are called the Hartree and the exchange potential, respectively. What makes the solution of Eq. 33 difficult is the fact that these potentials are not a priori known, but they rather depend on the functions  $\varphi_{\alpha\sigma}(\mathbf{x})$  to be determined,

$$V_{H}(\mathbf{x}) = \int d^{3}\mathbf{y}V(\mathbf{x}-\mathbf{y})\sum_{\alpha\sigma}|\varphi_{\alpha\sigma}(\mathbf{x})|^{2},$$
  
$$V_{\sigma}(\mathbf{x}-\mathbf{y}) = \sum_{\alpha}\varphi_{\alpha\sigma}^{*}(\mathbf{y})V(\mathbf{x}-\mathbf{y})\varphi_{\alpha\sigma}(\mathbf{x}),$$

where the sums are to be taken over occupied states. The Hartree potential is easily seen to describe the (classical) average potential created by all the particles in the system, whereas the exchange potential (which depends on the spin orientation in general) represents a quantum mechanical correction discovered by Fock. Note that the exchange potential is a non-local object, which greatly complicates the solution of Eq. 33. Usually the Hartree-Fock equations can be solved only numerically by an iterative method: first try a set of orbitals, then calculate the potentials, then solve for the new orbitals using these potentials. The calculation can be stopped when the old and new orbitals do not differ any more.

EXERCISE Show that  $H_{HF}$  is a hermitian operator.

Since  $H_{HF}$  is hermitian, its eigenvectors can be chosen orthogonal to each other, thereby forming an orthonormal set of states.

Taking the integral of Eq. 33, one finds readily that the single-particle energies can be written as

$$\varepsilon_{\alpha\sigma} = \int d^{3}\mathbf{x}\varphi_{\alpha\sigma}^{*}(\mathbf{x})H_{0}\varphi_{\alpha\sigma}(\mathbf{x}) + \sum_{\beta\sigma'}\int d^{3}\mathbf{x}\int d^{3}\mathbf{y}\varphi_{\alpha\sigma}^{*}(\mathbf{x})\varphi_{\beta\sigma'}^{*}(\mathbf{y})V(\mathbf{x}-\mathbf{y})\left[\varphi_{\beta\sigma'}(\mathbf{y})\varphi_{\alpha\sigma}(\mathbf{x}) - \delta_{\sigma\sigma'}\varphi_{\alpha\sigma}(\mathbf{y})\varphi_{\beta\sigma'}(\mathbf{x})\right].$$

Note that there is no factor 1/2 in the term coming from interactions. This means that the total energy of the system is not a simple sum of the single-particle energies  $\varepsilon_{\alpha\sigma}$ , but rather

$$E = \sum_{\alpha\sigma} \varepsilon_{\alpha\sigma} - \frac{1}{2} \sum_{\alpha\sigma} \sum_{\beta\sigma'} (\langle \alpha\beta | V | \alpha\beta \rangle - \delta_{\sigma\sigma'} \langle \alpha\beta | V | \beta\alpha \rangle),$$

where the sums are once again taken over the occupied states.

As a simple example of the Hartree-Fock method, consider the hydrogen molecule 'in an external field', described by the Hamiltonian

$$H = -t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}) + \Delta(n_2 - n_1).$$
(34)

The new term proportional to  $\Delta$  describes the action of the electric field: the energy at site 2 is  $+\Delta$ , whereas at site 1 it is  $-\Delta$ . This new term breaks the symmetry of the system with respect to parity, and therefore the exact solution (in the singlet sector) would require diagonalization of a 3 × 3 matrix. (Let us note in passing that the energy of the triplet states is not changed by the  $\Delta$  term.)

In order to proceed, let us assume that  $|\Psi\rangle = d^{\dagger}_{\uparrow}d^{\dagger}_{\downarrow}|0\rangle$  is the Slater determinant we are looking for. In other words, we assume that both the up-spin and the down-spin electrons occupy the same orbital  $d^{\dagger}|0\rangle = \varphi_1 c_1^{\dagger}|0\rangle + \varphi_2 c_2^{\dagger}|0\rangle$ , i.e. site *i* is occupied with probability amplitude  $\varphi_i$ . Obviously,  $\varphi_1$  and  $\varphi_2$  play the role of the wavefunction in our model.

EXERCISE Write down the Hartree-Fock equations for  $\varphi_1$  and  $\varphi_2$ . Solve the equations in the limits U = 0 and  $U \to \infty$ . Calculate the difference  $\delta$  of average occupations at sites 2 and 1. How does  $\delta$  change under increasing U? Why?

# LECTURE 4: JELLIUM MODEL-GROUND STATE PROPERTIES

### Jellium model

Now we are in the position to discuss the physics of many body systems. Let us start with the simplest model of a metal, the jellium model. This is a model of a metal in which the positive ion charge is smeared homogeneously in the volume of the crystal. The average charge densities of electrons and ions are equal in magnitude and of opposite sign, so as to make the crystal electrically neutral. The Hamiltonian of the system

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_{i}^{2}}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^{2}}{4\pi\epsilon_{0} |\mathbf{r}_{i} - \mathbf{r}_{j}|} + H_{ei} + H_{ii}$$

consists of a sum of kinetic energies of the electrons and of the Coulomb interaction energy among the electrons. The last two terms describe electron-ion and ion-ion Coulomb interactions, respectively.

We have an infinite system in mind, but in order to keep a countable basis set, we consider N electrons in a large box  $L \times L \times L$  with periodic boundary conditions. We take the system of plane waves  $|\mathbf{k}\rangle$  as our complete orthonormal set of one-particle (orbital) wavefunctions. In x-representation this basis reads  $\varphi_{\mathbf{k}}(\mathbf{x}) = L^{-3/2} \exp i \mathbf{k} \cdot \mathbf{x}$ . The wavenumber  $\mathbf{k}$  can take on the values  $(l, m, n)2\pi/L$ , where l, m, n are integers. The single-electron basis consists of a direct product  $|\mathbf{k}\sigma\rangle$  of the orbital basis and the spin basis  $|\sigma\rangle$ , the latter consisting of two states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

Transforming the Hamiltonian to the second quantized form, we first note that it does not depend on spin and therefore both nontrivial terms are diagonal in the spin index. Furthermore we note that  $\langle \mathbf{k} | \mathbf{p}^2 / 2m | \mathbf{k}' \rangle = \varepsilon_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'}$  with  $\varepsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$  and

$$\langle \mathbf{k_1} \mathbf{k_2} | \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} | \mathbf{k_3} \mathbf{k_4} \rangle = \frac{1}{\Omega} \delta_{\mathbf{k_1} + \mathbf{k_2}, \mathbf{k_3} + \mathbf{k_4}} V_{\mathbf{k_1} - \mathbf{k_3}},$$

where  $\Omega = L^3$  is the volume of the system and  $V_{\mathbf{q}} = \int d^3 \mathbf{r} (e^2/4\pi\epsilon_0 r) \exp i\mathbf{q} \cdot \mathbf{r}$  is the Fourier transform of the Coulomb potential. Therefore the Hamiltonian reads

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2\Omega} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}\neq 0} \sum_{\sigma,\sigma'} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}.$$
 (35)

Note that the Coulomb interaction energy does not contain the term with  $\mathbf{q} = 0$ . Moreover, neither  $H_{ei}$  nor  $H_{ii}$  enter Eq. 35. This is because the  $\mathbf{q} = 0$  term contributes an additive constant  $V_0N(N-1)/(2\Omega) \approx V_0N^2/(2\Omega)$  (the latter expression is valid if we consider only terms which are proportional to the volume of the system). This constant is precisely cancelled by the Coulomb interactions with (and within) the background.

EXERCISE Show that  $V_{\mathbf{q}} = e^2/(\varepsilon_0 \mathbf{q}^2)$ . Hint. Making use of contour integration, show that

$$\int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{e^{-i\mathbf{q}\cdot\mathbf{r}}}{(\mathbf{q}^2 + k_s^2)} = \frac{e^{-k_s r}}{4\pi r}$$
(36)

and take the limit  $k_s \to 0$ .

#### Free electron gas

In what follows we treat the jellium model Eq. 35 within perturbation theory. We take the kinetic energy as the unperturbed part of the Hamiltonian and the Coulomb interaction term is considered as a small perturbation. We will see that this perturbative approach is justified in the limit of a dense electron gas.

We start with the unperturbed Hamiltonian corresponding to a noninteracting electron gas. Due to the Pauli principle, not all electrons can occupy the lowest energy state with  $\mathbf{k} = 0$ . Rather, the electrons fill all  $|\mathbf{k}\sigma\rangle$  states with  $k < k_F$ , where  $k_F$  is the so-called Fermi wavevector. The occupied region of **k**-space is called the Fermi sea and the surface dividing the occupied and unoccupied regions is called the Fermi surface. The ground state wavefunction can be written

$$|FS\rangle = \prod_{|\mathbf{k}| < k_F} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}\downarrow} |0\rangle.$$
(37)

For the sake of simplicity, we assume that N satisfies the so-called closed-shell condition, which states that if there are several  $|\mathbf{k}\rangle$  vectors with the same energy, all of them are either simultaneously full, or simultaneously empty. Under these conditions the ground state is unique and its total spin S = 0 and total momentum  $\mathbf{P} = 0$ .

The Fermi surface encloses a volume  $(4/3)\pi k_F^3$ , inside of which there is a grid of occupied  $|\mathbf{k}\rangle$  states. Each of these states has an associated volume  $(2\pi/L)^3$  and is occupied with two electrons, one with spin up and the other with spin down. Therefore the total number of electrons is equal to  $k_F^3\Omega/(3\pi^2)$ . Equating this number with N we find an expression for the Fermi wavevector,  $k_F = (3\pi^2 n)^{1/3}$ , where  $n = N/\Omega$  is the density of electrons. Therefore the maximal energy of occupied states (the so-called Fermi energy) is  $\varepsilon_F = \hbar^2 k_F^2/(2m)$ .

EXERCISE Show that the total ground state energy of a noninteracting Fermi gas is  $E_0/N = (3/5)\varepsilon_F$ . Hint. In the limit of a large system  $L \to \infty$ , sums over k-space can be approximated by integrals,  $\Omega^{-1} \sum_{\mathbf{k}} \to (2\pi)^{-3} \int d^3 \mathbf{k}$ .

It is useful to associate with each electron a ball with radius  $r_0$  such that  $n = [(4/3)\pi r_0^3]^{-1}$ . Then the typical distance between nearby electrons is of the order  $r_0$ . In what follows we will sometimes characterize the electron gas by a dimensionless ratio  $r_s = r_0/a_B$  and measure lengths in units of the Bohr radius  $a_B = 4\pi\epsilon_0\hbar^2/(me^2)$  and energy in units of  $E_B = \hbar^2/(2ma_B^2)$ . In these units the ground state energy of the Fermi gas reads  $E_0/(NE_B) = 2.21/r_s^2$ . Note that  $E_0 \propto k_F^2 \propto r_s^{-2}$ .

# Perturbation theory: first order

Next we discuss the first-order correction to the ground-state energy  $E = E_0 + E_1 + \ldots$ ,

$$E_1 = \frac{1}{2\Omega} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}\neq 0} \sum_{\sigma,\sigma'} \frac{e^2}{\epsilon_0 \mathbf{q}^2} \langle FS | c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} | FS \rangle,$$

where  $|FS\rangle$  is the unperturbed ground state. The matrix element yields a finite contribution only if the operator  $c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'}$  creates the same two single particle states which were annihilated by the operator  $c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}$ . Since  $\mathbf{q} \neq 0$ , this is possible only if  $\mathbf{k} = \mathbf{k}' - \mathbf{q}$  and  $\sigma = \sigma'$ . Therefore  $E_1$  simplifies to

$$E_1 = \frac{1}{2\Omega} \sum_{\mathbf{k}' \neq \mathbf{k}} \sum_{\sigma} \frac{e^2}{\epsilon_0 (\mathbf{k}' - \mathbf{k})^2} \langle FS | c^{\dagger}_{\mathbf{k}'\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} | FS \rangle = -\frac{1}{\Omega} \sum_{\mathbf{k}' \neq \mathbf{k}} \frac{e^2}{\epsilon_0 (\mathbf{k}' - \mathbf{k})^2} f_{\mathbf{k}} f_{\mathbf{k}'},$$

where we have denoted the occupation number of the one-particle state  $|\mathbf{k}\sigma\rangle$  in the many particle wavefunction Eq. 37 as  $f_{\mathbf{k}}$ . (Note that we have made explicit use of the fact that  $c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|FS\rangle = f_{\mathbf{k}}|FS\rangle$ , irrespective of the value of  $\sigma$ .) Also note that  $f_{\mathbf{k}}$  is a simple step function,  $f_{\mathbf{k}} = 1$  for  $|\mathbf{k}| < k_F$  and  $f_{\mathbf{k}} = 0$  otherwise. Changing the summation variables and replacing the sums by integrals we obtain

$$E_1 = -\frac{1}{\Omega} \sum_{\mathbf{q}\neq 0,\mathbf{k}} \frac{e^2}{\epsilon_0 \mathbf{q}^2} f_{\mathbf{k}} f_{\mathbf{k}-\mathbf{q}} = -\frac{\Omega e^2}{\epsilon_0 (2\pi)^3} \int \frac{d^3 \mathbf{q}}{\mathbf{q}^2} F(\mathbf{q}), \tag{38}$$

where we have introduced  $F(\mathbf{q}) = (2\pi)^{-3} \int d^3 \mathbf{k} f_{\mathbf{k}} f_{\mathbf{k}-\mathbf{q}}$ . The function  $F(\mathbf{q})$  can be interpreted as the volume of the intersection of two identical Fermi spheres displaced by  $\mathbf{q}$ , see

Fig. 1. One finds readily that

$$F(\mathbf{q}) = \frac{3n}{4} \left[ \frac{2}{3} - \frac{q}{2k_F} + \frac{1}{3} \left( \frac{q}{2k_F} \right)^2 \right]$$

for  $q = |\mathbf{q}| < 2k_F$  and zero otherwise.



Figure 1: Left: the region in **k**-space whose volume defines the function  $F(\mathbf{q})$ . Right: the correlation function g(R).

The integration over  $\mathbf{q}$  in Eq. 38 can be performed trivially in spherical coordinates. Summarizing we find that the ground state energy is, to first order in interaction energy,

$$\frac{E}{N} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} - \frac{3}{16\pi^2} \frac{e^2 k_F}{\epsilon_0},$$
  
$$\frac{E}{NE_B} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s}.$$
 (39)

From the second form of Eq. 39 one can see that in the low-density limit  $r_s \ll 1$ , the kinetic energy per one particle is much larger than the interaction energy. It is therefore in this limit where our perturbative calculation is valid. Before proceeding it is worth pointing out that for electrons in simple metals,  $r_s$  lies in the range between 1.8 and 5.6. The applicability of perturbation theory to metals is therefore highly nontrivial.

### Correlations within the Fermi sea

The fact that  $E_1 < 0$  indicates that already within the wavefunction Eq. 37, the electrons avoid each other, which lowers the energy of the system. In order to clarify this issue, let us first define the density operator in point  $\mathbf{r}$ ,  $\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i)$ . Alternatively, in second quantization we can write  $\rho(\mathbf{r}) = \Omega^{-1} \sum_{\mathbf{k},\mathbf{q},\sigma} \exp(i\mathbf{q}\cdot\mathbf{r})c^{\dagger}_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{k}\sigma}$ . Note that, making use of this second quantized form, the expectation value of  $\rho(\mathbf{r})$  in the Fermi sea is easily seen to be  $\langle FS | \rho(\mathbf{r}) | FS \rangle = N/\Omega = n$ , proving explicitly the translational invariance of the system.

Let us compute the function  $g(\mathbf{R})$  defined as

$$n^{2}g(\mathbf{R}) = \langle FS|\rho(0)\rho(\mathbf{R})|FS\rangle - n\delta(\mathbf{R}) = \frac{1}{\Omega} \int d^{3}\mathbf{r} \langle FS|\rho(\mathbf{r})\rho(\mathbf{r}+\mathbf{R})|FS\rangle - n\delta(\mathbf{R}), \quad (40)$$

where in the second equation we have made use of the translational invariance of the system. Note that for large  $\mathbf{R}$  one expects that the density at point  $\mathbf{r} + \mathbf{R}$  is not affected by

its value at **r** and therefore  $\langle FS|\rho(\mathbf{r})\rho(\mathbf{r}+\mathbf{R})|FS\rangle \approx \langle FS|\rho(\mathbf{r})|FS\rangle\langle FS|\rho(\mathbf{r}+\mathbf{R})|FS\rangle = n^2$ . In other words, at large distances the function  $g(\mathbf{R}) \approx 1$ .

In order to clarify the physical meaning of  $g(\mathbf{R})$ , let us insert for  $\rho(\mathbf{r})$  its first quantized definition and perform the integral over  $\mathbf{r}$ . Then we find

$$n^2 g(\mathbf{R}) = \frac{1}{\Omega} \sum_{i \neq j} \langle FS | \delta(\mathbf{r_j} - \mathbf{r_i} - \mathbf{R}) | FS \rangle,$$

showing explicitly that  $g(\mathbf{R})$  is proportional to the probability of finding two electrons at a relative distance  $\mathbf{R}$ . Functions of the type Eq. 40, where expectation values of local quantities at different points are considered, are called correlation functions in the literature.

The correlation function Eq. 40 can be evaluated by going over to second quantization, which way we find  $n^2 g(\mathbf{R}) = n^2 - 2(2\pi)^{-3} \int d^3 \mathbf{q} F(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}}$ . Note that the same function  $F(\mathbf{q})$  enters both, the first-order correction to energy and the correlation function.

EXERCISE: Performing the  $\mathbf{q}$  integration in spherical coordinates, show that

$$g(R) = 1 - \frac{9}{2} \left[ \frac{\cos k_F R - (k_F R)^{-1} \sin k_F R}{(k_F R)^2} \right]^2.$$

The function g(R) is plotted in Fig. 1. Note that the probability to find two different electrons at the same point is one half of the probability to find them far apart from each other. This is a consequence of the Pauli principle: one half of all electrons (namely that half which has the same spin as the chosen electron) is repelled from the test electron, while the other half (with opposite spin) does not feel the presence of the test electrons. The suppression of g(R) extends to distances  $\sim k_F^{-1}$ , i.e. it is on the order of a typical electron-electron spacing  $r_0$ . This suppression is called the exchange hole in the literature.

# Low electron densities: the Wigner crystal

In the limit of small electron densities, the potential energy is expected to dominate over the kinetic energy and, as pointed out long ago by Wigner, the electron gas should crystallize. In what follows we give a crude estimate of the ground state energy in this phase.

The crystal is a periodic collection of sites, around which the electron is localized. Each lattice site we view as a spherical region (with radius  $r_0$ ), within which there is one electron moving in a homogeneously distributed charge |e|. Outside this spherical region, there is an uncharged background (from the point of view of the chosen electron), see Fig. 2.

The ground state energy per electron can be estimated as a sum of the Coulomb energy of the ionic background  $\varepsilon_{ii}$  and of the energy  $\varepsilon$  of an electron moving in the potential generated by the background,  $E/N = \varepsilon_{ii} + \varepsilon$ .

EXERCISE Show that the electrostatic potential generated by a homogeneously charged sphere (with total charge |e| and radius  $r_0$ ) is  $\phi/\phi_0 = (3 - r^2/r_0^2)/2$  for  $r < r_0$  and  $\phi/\phi_0 = r_0/r$  for  $r > r_0$ , where  $\phi_0 = |e|/(4\pi\epsilon_0 r_0)$ . Hint: calculate the electric field **E** at radius r (using Gauss' law) and make use of  $\mathbf{E} = -\nabla\phi$ .



Figure 2: Left: the spherical cavity of positive charge inside an uncharged background (shaded region). Right: The electrostatic potential of a homogeneously charged sphere.

The ion-ion energy can be calculated as  $\varepsilon_{ii} = (|e|/2) \int d^3 \mathbf{r} \phi(\mathbf{r}) n$ , from where we obtain in atomic units  $\varepsilon_{ii}/E_B = 6/(5r_s)$ . On the other hand, the electron is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 - |e|\phi(\mathbf{r}),$$

which can be thought of as a sum of harmonic oscillators in x, y, and z directions. Therefore  $\varepsilon = 3\hbar\omega_0/2 - 3e^2/(8\pi\epsilon_0 r_0)$ , where  $\omega_0 = e/(4\pi\epsilon_0 r_0^3 m)^{1/2}$ . In atomic units we can write  $\varepsilon/E_B = 3/r_s^{3/2} - 3/r_s$  and therefore the total energy per electron in the Wigner crystal phase is

$$\frac{E}{NE_B} = \frac{3}{r_s^{3/2}} - \frac{1.8}{r_s}.$$

In Fig. 3 we compare the energy of the Wigner crystal with that of the electron gas, Eq. 39. As was to be expected, the energy in the crystalline phase is lower at large  $r_s$ .



Figure 3: Comparison of the ground-state energies of the jellium model. Solid line: Eq. 39. Dashed line: energy of the Wigner crystal.

EXERCISE The Wigner crystal is stable as long as the mean deviation of the harmonic oscillator is much less than  $r_0$ . Show that this is equivalent to the criterion  $r_s \gg 1$ .

# LECTURE 5: JELLIUM MODEL-ELEMENTARY EXCITATIONS

### Quasiparticle excitations

Now we turn to the discussion of elementary excitations of the jellium model. First let us consider a state with an added extra electron with momentum  $K > k_F$ ,

$$|\psi\rangle = c^{\dagger}_{\mathbf{K}\alpha}|FS\rangle.$$

The momentum of this state is  $\hbar \mathbf{K}$ , spin S = 1/2, and  $S^z = \alpha$ . These quantum numbers are identical to those of an electron in vacuum, but, due to the interactions with filled Fermi sea, the excitation energy of this state, i.e. the difference  $\tilde{\varepsilon}_{\mathbf{K}} = \langle \psi | H | \psi \rangle - \langle FS | H | FS \rangle$  is different from the energy of an electron in vacuum,  $\varepsilon_{\mathbf{K}}$ . In fact,

$$\begin{aligned} \langle \psi | H | \psi \rangle &= \varepsilon_{\mathbf{K}} - \frac{1}{2\Omega} \sum_{\mathbf{k} \neq \mathbf{k}'} \sum_{\sigma} V_{\mathbf{k} - \mathbf{k}'} \langle \psi | c^{\dagger}_{\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} | \psi \rangle, \\ &= \varepsilon_{\mathbf{K}} - \frac{1}{2\Omega} \sum_{\mathbf{k} \neq \mathbf{k}'} \sum_{\sigma} V_{\mathbf{k} - \mathbf{k}'} (f_{\mathbf{k}} + \delta_{\mathbf{k}\mathbf{K}} \delta_{\sigma\alpha}) (f_{\mathbf{k}'} + \delta_{\mathbf{k}'\mathbf{K}} \delta_{\sigma\alpha}). \end{aligned}$$

From here one finds easily that

$$\tilde{\varepsilon}_{\mathbf{K}} = \varepsilon_{\mathbf{K}} - \frac{1}{\Omega} \sum_{\mathbf{k}} V_{\mathbf{K}-\mathbf{k}} f_{\mathbf{k}} = \varepsilon_{\mathbf{K}} - \frac{e^2}{\epsilon_0} \int_{|\mathbf{k}| < k_F} \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{K^2 + k^2 - 2\mathbf{K} \cdot \mathbf{k}}.$$

EXERCISE Making use of integration in spherical coordinates, show that

$$\tilde{\varepsilon}_{\mathbf{K}} = \varepsilon_{\mathbf{K}} - \frac{e^2 k_F}{4\pi^2 \epsilon_0} F\left(\frac{K}{k_F}\right),$$
  
$$F(x) = \frac{1-x^2}{2x} \ln\left|\frac{1+x}{1-x}\right| + 1.$$

If we define the Fermi velocity as  $\mathbf{v}_{\mathbf{K}} = \hbar^{-1} \partial \tilde{\varepsilon}_{\mathbf{K}} / \partial \mathbf{K}$ , and if we introduce a Fermi velocity  $v_F = \hbar k_F / m$ , then in the vicinity of the Fermi surface we can write

$$\frac{v_K}{v_F} = 1 + Cr_s \ln \frac{2k_F}{|K - k_F|},$$

where  $C = \pi^{-1} (4/9\pi)^{1/3}$ . Note that in the limit of high densities  $r_s \ll 1$ , the correction term is small, except very close to the Fermi energy, where it diverges.

Two lessons can be learned from this simple example. The first is that within a correlated many body system, excitation energies of electrons are different from those in the vacuum. This was to be expected, however: when an electron is added to the electron liquid, it has to develop an exchange hole and the charge distribution in its vicinity is altered. Therefore, obviously, the electron energy is renormalized. Also in more advanced approximations we can usually talk about a particle and the deformation of the background which it causes. This composite object (bare particle+deformation of the reservoir) is called quasiparticle in the literature. Before proceeding let us point out

that the 'bare particle' in this scheme does not need to be an added particle. In fact, if we remove an electron with  $K < k_F$  from the Fermi sea,

$$|\psi'\rangle = c_{\mathbf{K}\alpha}|FS\rangle,$$

we can talk about a hole. The momentum of the state  $|\psi'\rangle$  is  $-\hbar \mathbf{K}$ , its spin is S = 1/2, and  $S^z = -\alpha$ .

The second lesson to be learned regards first-order perturbation theory: within that approximation, the quasiparticle velocity diverges at the Fermi surface, in gross disagreement with experiments. This indicates that the apparent success of perturbation theory for the ground state energy (at  $r_s \ll 1$ ) does not carry over to quasiparticle properties.

#### Random phase approximation

One can verify easily that the breakdown of low-order perturbation theory for  $\mathbf{v}_{\mathbf{K}}$  is caused by the long range character of the Coulomb force and the associated divergence of  $V_{\mathbf{q}}$  at  $q \rightarrow 0$ . What has gone wrong? In our calculation we have considered the unperturbed wavefunction  $|\psi\rangle$  in which it has not been taken into account that every test charge introduced into the electron liquid (and therefore every electron) will accumulate a screening charge of equal magnitude and opposite charge around itself, due to which process at distances larger than the size of the screening cloud the electric field due to the test charge is negligible. In what follows we therefore introduce a method which allows us to take this screening into account.

Let us consider that into the electron liquid, we insert a small test charge density

$$\frac{e}{\Omega} \left[ \rho_{\mathbf{q}}^{\text{ext}} \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t) + \rho_{-\mathbf{q}}^{\text{ext}} \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t) \right].$$

The electron system will screen this test charge density. In what follows we will see that if the perturbation is assumed to be small, the screening charge density will be given by

$$\frac{e}{\Omega} \left[ \rho_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t) + \rho_{-\mathbf{q}} \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t) \right].$$
(41)

Therefore the total charge density is given by

$$\frac{e}{\Omega} \left[ \rho_{\mathbf{q}}^{\text{tot}} \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t) + \rho_{-\mathbf{q}}^{\text{tot}} \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t) \right], \tag{42}$$

where  $\rho_{\mathbf{q}}^{\text{tot}} = \rho_{\mathbf{q}}^{\text{ext}} + \rho_{\mathbf{q}}$  and  $\rho_{-\mathbf{q}}^{\text{tot}} = \rho_{-\mathbf{q}}^{\text{ext}} + \rho_{-\mathbf{q}}$ , respectively. Since the electrostatic potential is related to the charge density through the Laplace equation,  $\nabla^2 \phi(\mathbf{r}) = -\epsilon_0^{-1} e \rho(\mathbf{r})$ , we can introduce three types of electrostatic potentials, all of which can be written as

$$\phi_{\mathbf{q}}^{i} \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t) + \phi_{-\mathbf{q}}^{i} \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t),$$

 $\phi^i_{\pm \mathbf{q}} = (\epsilon_0 \Omega q^2)^{-1} e \rho^i_{\pm \mathbf{q}}$  and the upper index *i* discriminates the external, induced, and total potentials. As usual in the theory of electromagnetism, we define now a dielectric function

$$\epsilon(\mathbf{q},\omega) = \frac{\phi_{\mathbf{q}}^{\text{ext}}}{\phi_{\mathbf{q}}^{\text{tot}}} = \frac{\rho_{\mathbf{q}}^{\text{ext}}}{\rho_{\mathbf{q}}^{\text{tot}}} = 1 - \frac{\rho_{\mathbf{q}}}{\rho_{\mathbf{q}}^{\text{tot}}},\tag{43}$$

where we have shown explicitly the wavevector and frequency dependence of the dielectric function. An alternative way of writing Eq. 43 is

$$\frac{1}{\epsilon(\mathbf{q},\omega)} = \frac{\phi_{\mathbf{q}}^{\text{tot}}}{\phi_{\mathbf{q}}^{\text{ext}}} = \frac{\rho_{\mathbf{q}}^{\text{tot}}}{\rho_{\mathbf{q}}^{\text{ext}}} = 1 + \frac{\rho_{\mathbf{q}}}{\rho_{\mathbf{q}}^{\text{ext}}}.$$
(44)

The form Eq. 44 is useful in fully microscopic formulations of the screening problem, which we do not attempt here.

So far, our treatment of screening was exact (in the limit of a vanishing  $\rho^{\text{ext}}$ ). Now we introduce the so-called random phase approximation (RPA), according to which  $\epsilon(\mathbf{q}, \omega)$  is calculated from Eq. 43 where the ratio  $\rho/\rho^{\text{tot}}$  is approximated by the response of a non-interacting electron gas to a perturbing charge density Eq. 42. The Hamiltonian for the electron system is  $H = H_{\text{kin}} + H'$ , where

$$H'(t) = e \int d^3 \mathbf{r} \hat{\rho}(\mathbf{r}) \phi^{\text{tot}}(\mathbf{r}) = \frac{e^2}{\epsilon_0 \Omega q^2} \left[ \hat{\rho}_{-\mathbf{q}} \rho_{\mathbf{q}}^{\text{tot}} e^{-i\omega t} + \hat{\rho}_{\mathbf{q}} \rho_{-\mathbf{q}}^{\text{tot}} e^{i\omega t} \right] e^{\eta t},$$

where, in order to distinguish expectation values and operators, we have introduced hats for the latter. In particular,  $\hat{\rho}(\mathbf{r})$  is the operator of electron density and  $\hat{\rho}_{\mathbf{q}} = \sum_{i=1}^{N} \exp(-i\mathbf{q} \cdot \mathbf{r}_i)$  is its Fourier transform. We have introduced into H' also a factor  $\exp(\eta t)$  where it is understood that  $\eta$  is small and will be set zero at the end of the calculation. Its physical meaning is that it corresponds to a slow switching on of the perturbation, since  $\exp(\eta t) = 0$  for  $t \to -\infty$  and  $\exp(\eta t) = 1$  for t = 0.

Let us solve now the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \left[H_{\rm kin} + H'(t)\right] |\Psi\rangle$$

making use of time-dependent perturbation theory, assuming that at  $t = -\infty$ , the system was in the ground state of  $H_{\rm kin}$ . To this end, we expand  $|\Psi(t)\rangle$  in a set of eigenstates  $|n\rangle$ of  $H_{\rm kin}$ ,

$$|\Psi(t)\rangle = \sum_{n} a_n(t) e^{-iE_n t/\hbar} |n\rangle,$$

where  $E_n$  is the energy of state  $|n\rangle$ . Note that  $|n\rangle$  is a time-independent basis state in the Heisenberg picture, whereas  $|\Psi(t)\rangle$  is a state in the Schrödinger picture. The expansion coefficients have to satisfy the boundary condition  $a_0(-\infty) = 1$  and  $a_n(-\infty) = 0$  for all excited states.

EXERCISE Show that standard time-dependent perturbation theory leads to the result  $a_0(t) = 1$  and, for  $n \neq 0$ ,

$$a_n(t) = -\frac{e^2}{\hbar\epsilon_0 \Omega q^2} \left[ \frac{\langle n|\hat{\rho}_{-\mathbf{q}}|0\rangle \rho_{\mathbf{q}}^{\text{tot}}}{\omega_{n0} - \omega - i\eta} e^{i(\omega_{n0} - \omega - i\eta)t} + \frac{\langle n|\hat{\rho}_{\mathbf{q}}|0\rangle \rho_{-\mathbf{q}}^{\text{tot}}}{\omega_{n0} + \omega - i\eta} e^{i(\omega_{n0} + \omega - i\eta)t} \right],$$

where  $\omega_{n0} = (E_n - E_0)/\hbar$ .

To first order in  $\rho^{\text{tot}}$ , the expectation value of  $\hat{\rho}_{\mathbf{q}}$  in the state  $|\Psi(t)\rangle$  reads

$$\begin{aligned} \langle \Psi(t) | \hat{\rho}_{\mathbf{q}} | \Psi(t) \rangle &= \langle \Psi(t) | \hat{\rho}_{\mathbf{q}} | 0 \rangle e^{-iE_0 t/\hbar} + \langle 0 | \hat{\rho}_{\mathbf{q}} | \Psi(t) \rangle e^{iE_0 t/\hbar} \\ &= \sum_{n \neq 0} \left[ a_n(t) e^{-i\omega_{n0} t} \langle 0 | \hat{\rho}_{\mathbf{q}} | n \rangle + a_n^*(t) e^{i\omega_{n0} t} \langle n | \hat{\rho}_{\mathbf{q}} | 0 \rangle \right]. \end{aligned}$$

Making use of the second-quantized form  $\hat{\rho}_{\mathbf{q}} = \sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}$ , one can see readily that  $\langle n|\hat{\rho}_{\mathbf{q}}|0\rangle$  is finite only if the momentum of the state  $|n\rangle$  is  $-\hbar\mathbf{q}$ . For this state obviously  $\langle n|\hat{\rho}_{-\mathbf{q}}|0\rangle = 0$ . Moreover, note that  $\langle 0|\hat{\rho}_{\mathbf{q}}|n\rangle = \langle n|\hat{\rho}_{-\mathbf{q}}|0\rangle^*$ . After a simple calculation we find then

$$\langle \Psi(t)|\hat{\rho}_{\mathbf{q}}|\Psi(t)\rangle = -\frac{e^2}{\hbar\epsilon_0\Omega q^2}\rho_{\mathbf{q}}^{\text{tot}}e^{-i\omega t+\eta t}\sum_{n\neq 0}\left[\frac{|\langle n|\hat{\rho}_{-\mathbf{q}}|0\rangle|^2}{\omega_{n0}-(\omega+i\eta)} + \frac{|\langle n|\hat{\rho}_{\mathbf{q}}|0\rangle|^2}{\omega_{n0}+(\omega+i\eta)}\right]$$

Thus the induced charge has precisely the same form as expected in Eq. 41 and we can calculate the dielectric function making use of Eq. 43. We obtain

$$\epsilon(\mathbf{q},\omega) = 1 + V_{\mathbf{q}}\chi(\mathbf{q},\omega),\tag{45}$$

where the so-called polarization  $\chi(\mathbf{q}, \omega)$  reads

$$\chi(\mathbf{q},\omega) = \frac{1}{\hbar\Omega} \sum_{n\neq 0} |\langle n|\hat{\rho}_{\mathbf{q}}|0\rangle|^2 \left[\frac{1}{\omega_{n0} - (\omega + i\eta)} + \frac{1}{\omega_{n0} + (\omega + i\eta)}\right].$$

In arriving at this expression we have assumed that the system is invariant by reflection. In fact, the states  $|n\rangle$  contributing to the sum in the first term of  $\chi(\mathbf{q}, \omega)$  and the states  $|n'\rangle$  contributing to the second term are related by reflection symmetry. In a symmetric system their energies are equal,  $E_n = E_{n'}$ , and therefore the simplification is justified.

Finally, let us note that the states  $|n\rangle$  which contribute to  $\chi(\mathbf{q}, \omega)$  can be fully described by specifying the wavevector  $\mathbf{k}$  and spin  $\sigma$  of the state to be created. Therefore we have  $|\langle n|\hat{\rho}_{\mathbf{q}}|0\rangle|^2 = f_{\mathbf{k}+\mathbf{q}}(1-f_{\mathbf{k}})$  and

$$\chi(\mathbf{q},\omega) = \frac{2}{\Omega} \sum_{\mathbf{k}} f_{\mathbf{k}+\mathbf{q}} (1-f_{\mathbf{k}}) \left[ \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} - (\hbar\omega + i\hbar\eta)} + \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} + (\hbar\omega + i\hbar\eta)} \right].$$

where the factor of two comes from summation over spins. By making the dummy variable transformation  $\mathbf{k} \to -\mathbf{k} - \mathbf{q}$  in the second term and making use of the assumed reflection symmetry  $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$  we finally find

$$\chi(\mathbf{q},\omega) = \frac{2}{\Omega} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} - \hbar\omega - i\hbar\eta}.$$
(46)

### Static screening of Coulomb interactions

Now we are in the position to discuss screening. We consider the static case, when  $\omega = 0$  and the susceptibility at small **q** reads

$$\chi(\mathbf{q},0) = -\frac{2}{\Omega} \sum_{\mathbf{k}} \frac{df}{d\varepsilon} = \frac{2}{(2\pi)^3} \int d^3 \mathbf{k} \,\delta\left[\frac{\hbar^2}{2m} (\mathbf{k}^2 - k_F^2)\right] = \frac{mk_F}{\pi^2 \hbar^2}.$$

Here we have taken into account that the derivative of a step function is a Dirac delta function. Inserting the expression for  $\chi(\mathbf{q}, 0)$  into the dielectric function, we find  $\epsilon(\mathbf{q}, 0) = 1 + k_s^2/q^2$ , where  $k_s^2 = me^2 k_F/(\epsilon_0 \pi^2 \hbar^2)$ . Therefore the Fourier transform of the static screened Coulomb interaction in the long-wavelength limit reads

$$V_{\mathbf{q}}^{s} = \frac{e^{2}}{\epsilon_{0}q^{2}\epsilon(\mathbf{q},0)} = \frac{e^{2}}{\epsilon_{0}(q^{2}+k_{s}^{2})}$$

Note that this interaction is not any more singular at  $q \to 0$ . Moreover, as Eq. 36 shows,  $k_s$  is the inverse screening length (the so-called Thomas-Fermi screening length). When measured in units of  $k_F$ , the inverse screening length reads

$$\left(\frac{k_s}{k_F}\right)^2 = 4Cr_s,$$

where C is the same numerical constant which appeared in the renormalization of Fermi velocity. This result means that in the high-density limit  $r_s \ll 1$  the screening length scales like  $k_s^{-1} \propto a_B \sqrt{r_s}$ , i.e. it is much longer than the average interparticle distance  $a_B r_s$ .

# LECTURE 6

#### Collective excitations: plasmons

Another interesting physical effect which can be discussed making use of the dielectric function are the density oscillations of the electron gas, the so-called plasmons. Physically, the existence of such collective excitations can be explained as follows. Imagine that at some space-time point the density of the electrons diminishes for some reason. The electron liquid will flow towards this region, in order to restore charge neutrality, but, because of inertial effects, the screening electrons overshoot. Thus the initial charge fluctuation is not screened and the process of screening starts again.

From the formal point of view, spontaneous oscillations of density are expected whenever  $\epsilon(\mathbf{q}, \omega) = 0$ . This can be seen from Eq. 43 which can be written in the form  $\phi^{\text{tot}} = \phi^{\text{ext}}/\epsilon(\mathbf{q}, \omega)$ . This means that even if the external potential  $\phi^{\text{ext}}$  vanishes, there can still be a finite total internal field  $\phi^{\text{tot}}$ .

EXERCISE Show that in the limit when  $\mathbf{q} \to 0$  and  $\omega$  is finite,

$$\chi(\mathbf{q},\omega) = -\frac{2}{\Omega\hbar^2\omega^2}\sum_{\mathbf{k}} f_{\mathbf{k}}(\varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}-\mathbf{q}} - 2\varepsilon_{\mathbf{k}}) = -\frac{nq^2}{m\omega^2}.$$

From here it follows that  $\epsilon(0,\omega) = 1 - \omega_p^2/\omega^2$  where we have introduced  $\omega_p^2 = ne^2/(m\epsilon_0)$ . Since the dielectric function vanishes for  $\omega = \omega_p$ , one can see that  $\omega_p$  is the frequency of spontaneous plasma oscillations. It is called plasma frequency in the literature.

## Plasmons - alternative derivation

Note that in the formula for  $\omega_p$  there is no  $\hbar$ . This is in agreement with the fact that the notion of plasma oscillations can be derived also from purely classical considerations. In fact, let us assume small density oscillations of the electron gas described by the electron density  $\rho(\mathbf{r})$ . The continuity equation reads

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0,$$

where  $\mathbf{j} = n\mathbf{v}$  is the electron current density (note that since we keep only lowest-order terms, we have written in the expression for  $\mathbf{j}$  the average electron density n instead of

 $\rho$ ). Plasma oscillations will lead to appearance of an electric field **E** in the electron gas, which will accelerate the electrons,  $\partial \mathbf{v}/\partial t = e\mathbf{E}/m$ , and therefore

$$\frac{\partial \mathbf{j}}{\partial t} = \frac{ne}{m} \mathbf{E}.$$

Now, let us take the time derivative of the continuity equation and the quantity  $\partial (\nabla \cdot \mathbf{j}) / \partial t$  express by taking the divergence of the acceleration equation. In the result let us make use of the Maxwell equation  $\nabla \cdot \mathbf{E} = e\rho/\epsilon_0$ . This way we obtain

$$\frac{\partial^2 \rho}{\partial t^2} + \omega_p^2 \rho = 0, \tag{47}$$

showing explicitly that the electron gas supports plasma oscillations.

In what follows we construct a quantum-mechanical analogue of the above quasiclassical equations. This will be done by the method of equations of motion, i.e. from now we work in the Heisenberg picture. Our goal is to find an equation of motion for a long-wavelength density oscillation, which is described by the operator  $\rho_{\mathbf{q}}$ .

Let us first calculate the time derivative of  $\rho_{\mathbf{q}}$ ,

$$\frac{d\rho_{\mathbf{q}}}{dt} = \frac{i}{\hbar} [H, \rho_{\mathbf{q}}] = i \sum_{i=1}^{N} e^{-i\mathbf{q}\cdot\mathbf{r}_{i}} \left(\frac{\hbar q^{2}}{2m} - \frac{\mathbf{q}\cdot\mathbf{p}_{i}}{m}\right).$$
(48)

The calculation can be easily performed in the first-quantized form, since the Coulomb energy obviously commutes with  $\rho_{\mathbf{q}}$ . Therefore only the commutator of kinetic energy with  $\rho_{\mathbf{q}}$  has to be calculated. A useful identity enabling us to check Eq. 48 is

$$\frac{i}{\hbar} \left[ \frac{\mathbf{p}_i^2}{2m}, e^{-i\mathbf{q}\cdot\mathbf{r}_j} \right] = i \left[ \frac{\hbar q^2}{2m} - \frac{\mathbf{p}_i \cdot \mathbf{q}}{m} \right] \delta_{ij}$$

Note that Eq. 48 is the Fourier transform of a quantum-mechanical continuity equation, since it can be written as  $d\rho_{\mathbf{q}}/dt = -i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}}$ , where

$$\mathbf{j}_{\mathbf{q}} = \frac{1}{2} \sum_{i=1}^{N} \left[ e^{-i\mathbf{q}\cdot\mathbf{r}_{i}} \mathbf{v}_{i} + \mathbf{v}_{i} e^{-i\mathbf{q}\cdot\mathbf{r}_{i}} \right]$$

is the current density operator and  $\mathbf{v}_i = \mathbf{p}_i/m$  is the one-particle velocity operator.

In analogy with the classical solution, in the next step we have to calculate the time derivative of the operator  $d\rho_{\mathbf{q}}/dt$ :

$$\frac{d^2 \rho_{\mathbf{q}}}{dt^2} = \frac{i}{\hbar} \left[ H, \frac{d\rho_{\mathbf{q}}}{dt} \right] = -\sum_{i=1}^N e^{-i\mathbf{q}\cdot\mathbf{r}_i} \left[ \frac{\hbar q^2}{2m} - \frac{\mathbf{p}_i \cdot \mathbf{q}}{m} \right]^2 - \frac{1}{\Omega} \sum_{\mathbf{Q} \neq 0} V_{\mathbf{Q}} \frac{\mathbf{q} \cdot \mathbf{Q}}{m} \rho_{\mathbf{q}-\mathbf{Q}} \rho_{\mathbf{Q}}. \tag{49}$$

The first term in Eq. 49 comes from the commutation with the kinetic energy. The second term is a commutator with the Coulomb energy. This term is nonvanishing, because the operator  $d\rho_{\mathbf{q}}/dt$  contains also single-particle momentum operators. In arriving at Eq. 49, we have written the Coulomb interaction energy in the form

$$H_{\text{Coul}} = \frac{1}{2\Omega} \sum_{\mathbf{Q}\neq 0} V_{\mathbf{Q}}(\rho_{\mathbf{Q}}\rho_{-\mathbf{Q}} - N),$$

which can be proven easily if one inserts the second quantized form of  $\rho_{\mathbf{Q}}$  and compares with Eq. 35. In the derivation of Eq. 49, the commutation relation  $[\mathbf{p}_i, \rho_{\mathbf{Q}}] = -\hbar \mathbf{Q} e^{-i\mathbf{Q}\cdot\mathbf{r}_i}$ is useful.

Now we observe that on the right-hand side of Eq. 49 the first term is small in the limit  $\mathbf{q} \to 0$ . Moreover, the second term on the right-hand side is dominated by the contribution of  $\mathbf{Q} = \mathbf{q}$ , which yields  $\omega_p^2 \rho_{\mathbf{q}}$ . This is because for the remaining  $\mathbf{Q}$  vectors the wavevector of the density dluctuation can't be equal to zero (note that  $\mathbf{Q} = 0$  is not included in the sum). Note that  $\rho_{\mathbf{q}=0} = N$  is a macroscopic number, whereas for nonzero wavevectors the phases in  $\rho_{\mathbf{q}} = \sum_{i=1}^{N} \exp(-i\mathbf{q} \cdot i)$  vary randomly (for a high density electron gas, where the kinetic energy dominates) and are therefore likely to nearly cancel each other. In other words,  $\rho_{\mathbf{q}}$  for a high density electron gas is expected to be small. Neglecting the small terms we finally arrive at an equation for  $\rho_{\mathbf{q}}$  of the same form as Eq. 47. Hence, we have rederived the plasmon within a quantum-mechanical language.

#### Quasiparticle lifetime

Let us address the question whether, if we prepare a quasiparticle excitation with a given momentum and energy, the quasiparticle state remains unchanged for an infinitely long time. The answer to this question is obviuosly no, since e.g. a quasiparticle with  $k > k_F$ can scatter from  $\mathbf{k}\sigma$  to  $\mathbf{k} - \mathbf{q}\sigma$  by exciting a particle from an originally occupied state  $\mathbf{p}\sigma'$ below the Fermi level to an originally empty state  $\mathbf{p} + \mathbf{q}\sigma'$  outside the Fermi sea. The resulting hole in the state  $\mathbf{p}\sigma'$  and the particle in the state  $\mathbf{p} + \mathbf{q}\sigma'$  are called an excited particle-hole pair.



Figure 4: Scattering process leading to a finite lifetime of the electron.

In what follows we determine the quasiparticle lifetime  $\tau_{\mathbf{k}}$  by means of the Fermi golden rule,

$$\frac{\hbar}{\tau_{\mathbf{k}}} = 2 \times 2\pi \sum_{\mathbf{q}} \left(\frac{V_{\mathbf{q}}^s}{\Omega}\right)^2 \sum_{\mathbf{p}} f_{\mathbf{p}} (1 - f_{\mathbf{p}+\mathbf{q}}) (1 - f_{\mathbf{k}-\mathbf{q}}) \delta(\varepsilon_{\mathbf{k}-\mathbf{q}} + \varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{k}})$$

The Fermi functions make sure that the state  $\mathbf{p}$  is occupied and the states  $\mathbf{p} + \mathbf{q}$  and  $\mathbf{k} - \mathbf{q}$  are empty, the delta function takes into account the conservation of energy in the scattering process (note that momentum is conserved by definition), and the factor of 2 comes from a summation over  $\sigma'$ .

Let us consider only quasiparticles with low excitation energies, i.e. such which lie close to the Fermi level. Then it is easy to see that all four momenta involved in the scattering process have to be close to the Fermi level and because of this restriction we can replace the summations over momenta as follows

$$\frac{1}{\Omega}\sum_{\mathbf{p}} = \frac{1}{(2\pi)^3} \int d^3 \mathbf{k} = \frac{1}{(2\pi)^3} \int dk k^2 \int dS_k \approx N(0) \int d\varepsilon_k \int \frac{dS_k}{4\pi},$$

where  $\int dS_k$  is an angular integration in **k**-space and we have introduced the density of states at the Fermi level (for one spin direction)

$$N(0) = \frac{k_F^2}{2\pi^2 \hbar v_F} = \frac{mk_F}{2\pi^2 \hbar^2}.$$

Introducing  $\mathbf{k}' = \mathbf{k} + \mathbf{q}$  and  $\mathbf{p}' = \mathbf{p} - \mathbf{q}$  we can write the golden rule as a triple sum over  $\mathbf{p}$ ,  $\mathbf{p}'$ , and  $\mathbf{k}'$ , if we also introduce another three-dimensional delta function for momentum conservation. This way we obtain

$$\frac{\hbar}{\tau_{\mathbf{k}}} = 4\pi N(0)^3 \int \frac{dS_p}{4\pi} \int \frac{dS_{p'}}{4\pi} \int \frac{dS_{k'}}{4\pi} (V^s_{\mathbf{k'}-\mathbf{k}})^2 \delta(\mathbf{k'} + \mathbf{p'} - \mathbf{k} - \mathbf{p}) \\
\times \int d\varepsilon_p \int d\varepsilon_{p'} \int d\varepsilon_{k'} f_p (1 - f_{p'}) (1 - f_{k'}) \delta(\varepsilon_{k'} + \varepsilon_{p'} - \varepsilon_k - \varepsilon_p).$$
(50)

EXERCISE Show that the energy integral in the second line of Eq. 50 equals  $(\varepsilon_k - \varepsilon_F)^2/2$ . Hint. First introduce instead of  $\varepsilon$  its deviation from the Fermi level,  $\xi = \varepsilon - \varepsilon_F$ . Then show that the integral can be written as

$$\int_{-\infty}^{0} d\xi_p \int_0^{\infty} d\xi_{p'} \int_0^{\infty} d\xi_{k'} \delta(\xi_{k'} + \xi_{p'} - \xi_k - \xi_p) = \int_0^{\infty} d\xi_p \int_0^{\infty} d\xi_{p'} \int_0^{\infty} d\xi_{k'} \delta(\xi_p + \xi_{p'} + \xi_{k'} - \xi_k).$$

Show that the last integral equals  $\int_0^{\xi_k} d\xi_p \int_0^{\xi_k - \xi_p} d\xi_{p'}$ .

The angular integral in Eq. 50 can be shown to be finite. This then means that the inverse lifetime of a quasiparticle varies as  $\hbar/\tau_{\mathbf{k}} \propto (\varepsilon_k - \varepsilon_F)^2$ . Since, due to the Heisenberg uncertainty principle, a finite lifetime of a particle means a finite uncertainty of its energy  $\delta \varepsilon_{\mathbf{k}} \sim \hbar/\tau_{\mathbf{k}}$ , Eq. 50 implies that at sufficiently small excitation energies  $\varepsilon_k - \varepsilon_F$  the energy uncertainty of the quasiparticle becomes negligible with respect to the excitation energy of the quasiparticle, and therefore the very concept of a quasiparticle is well defined.