

Physics MSc of FNS BME  
I. Year, 1. semester

**MODERN SOLID STATE PHYSICS**  
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**Problem set**

1. Identical particles
2. Second quantization I. (bosons)
3. Second quantization II. (fermions)
4. Field operators
5. Phonons, magnons, bosons
6. Electrons I. (Fermi liquid, Hartree-Fock approximation, Wigner crystal)
7. Electrons II. (Wannier states, Hubbard model)
8. Condensates

## 1. Identical particles

- 1.1** Out of three bosons two is in the state  $\varphi_1(\mathbf{r})$ , while one is in the state  $\varphi_2(\mathbf{r})$ . Write down the symmetrized wavefunction  $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ , then calculate the normalization factor!
- 1.2** Prove that for  $N$  fermions the normalization factor of the antisymmetrized wavefunction is  $1/\sqrt{N!}$
- 1.3** Given  $N$  bosons
- prove that the normalization factor of the symmetrized wavefunction is  $\sqrt{N_1!N_2!\dots/N!}$ , if during the symmetrization we only take into account permutations leading to different terms!
  - what would be the normalization factor, if all permutations were included?
- 1.4** If the number of different states a particle can be in is  $\Omega$ , then the system of  $N$  such distinguishable particles can be in  $\Omega^N$  different states.
- How many physically different states can be occupied by a system of  $N$  fermions?
  - Suppose that  $\Omega = 2N$ . What is the asymptotics of the number of many body states of fermions and distinguishable particles for large  $N$ ?

## 2. Second quantization I.

- 2.1** Consider the three bosons of exercise 1.1.
- Using  $\psi_{112}$  determined there, calculate the expectation value of the operator  $F^{(1)} = f^{(1)}(\mathbf{r}_1) + f^{(1)}(\mathbf{r}_2) + f^{(1)}(\mathbf{r}_3)$  !
  - Determine the matrix element  $\langle \psi_{122} | F^{(1)} | \psi_{112} \rangle$ !
- 2.2** Prove the followings for  $N$  bosons and for the operator  $F^{(1)} = \sum_{i=1}^N f^{(1)}(\mathbf{r}_i)$
- $\langle \psi_{N_1, N_2, \dots} | F^{(1)} | \psi_{N_1, N_2, \dots} \rangle = \sum_j N_j f_{jj}^{(1)}$ .

b.  $\langle \psi_{\dots, N_j-1, \dots, N_k+1, \dots} | F^{(1)} | \psi_{\dots, N_j, \dots, N_k, \dots} \rangle = f_{kj}^{(1)} \sqrt{N_j(N_k+1)}$ .

**2.3** Consider a single one particle state, which can host arbitrary number of bosons.  $a^+$  and  $a$  are the usual creation and annihilation operators:

$$a|N\rangle = \sqrt{N}|N-1\rangle,$$

$$a^+|N\rangle = \sqrt{N+1}|N+1\rangle,$$

$$[a, a^+] = 1.$$

Calculate the following matrix elements between states with arbitrary  $N$  and  $N'$ :

a.  $\langle N' | a^+ a | N \rangle,$

b.  $\langle N' | a a^+ | N \rangle,$

c.  $\langle N' | a^+ a^+ | N \rangle,$

d.  $\langle N' | a a | N \rangle,$

e.  $\langle N' | a^+ a^+ a a | N \rangle,$

f.  $\langle N' | a^+ a a^+ a | N \rangle.$

**2.4** Consider several one particle states, which are filled by  $N_1, N_2, \dots$  bosons. The creation and annihilation operators corresponding to the  $j$ -th state are  $a_j^+$  and  $a_j$ . Calculate the following matrix elements:

a.  $\langle N_1, N_2, \dots | a_j^+ a_k | N_1, N_2, \dots \rangle,$

b.  $\langle \dots, N_j-1, \dots, N_k+1, \dots | a_l^+ a_m | \dots, N_j, \dots, N_k, \dots \rangle.$

**2.5** Utilizing the results of exercises 2.2 and 2.4 prove, that the second quantized form of the general one particle operator  $F^{(1)}$  is

$$F^{(1)} = \sum_{k,j} f_{kj}^{(1)} a_k^+ a_j.$$

**2.6\*** Utilizing the rules for bosons prove, that the second quantized form of the general two particle operator  $F^{(2)} = \sum_{i,j=1}^N f^{(2)}(\mathbf{r}_i, \mathbf{r}_j)$  is

$$F^{(2)} = \sum_{k,l,m,n} f_{klmn}^{(2)} a_k^+ a_l^+ a_m a_n,$$

where

$$f_{klmn}^{(2)} = \int d^3 r_1 \int d^3 r_2 \bar{\varphi}_k(\mathbf{r}_1) \bar{\varphi}_l(\mathbf{r}_2) f^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \varphi_m(\mathbf{r}_2) \varphi_n(\mathbf{r}_1).$$

### 3. Second quantization II.

**3.1** Prove that for  $N$  fermions the diagonal matrix elements of the one particle operator  $F^{(1)}$  are:

$$\langle N_1, N_2, \dots | F^{(1)} | N_1, N_2, \dots \rangle = \sum_j N_j f_{jj}^{(1)}.$$

**3.2** Prove that for  $N$  fermions the off diagonal matrix elements of the one particle operator  $F^{(1)}$  are:

$$\langle \dots, N_j - 1, \dots, N_k + 1, \dots | F^{(1)} | \dots, N_j, \dots, N_k, \dots \rangle = \pm f_{kj}^{(1)},$$

where  $N_j = 1$  and  $N_k = 0$  of course, moreover the sign of the right hand side is " + ", if there are an even number of particles in the states between states  $j$  and  $k$ , and " - ", if there are an odd number of particles in the states between states  $j$  and  $k$ .

**3.3** According to the definition of fermionic creation and annihilation operators:

$$a_k | \dots, N_k, \dots \rangle = (-1)^{\sum_{i < k} N_i} N_k | \dots, N_k - 1, \dots \rangle,$$

and

$$a_k^+ | \dots, N_k, \dots \rangle = (-1)^{\sum_{i < k} N_i} (1 - N_k) | \dots, N_k + 1, \dots \rangle.$$

Prove that

a.  $(a_k)^+ = a_k^+$ ,

b.  $a_k^+ a_k = N_k$ ,

c.  $a_i a_j^+ + a_j^+ a_i = \delta_{ij}$ .

**3.4**  $a_k$  and  $a_k^+$  are fermionic operators ( $k=1,2,\dots,5$ ). Calculate the following matrix elements:

a.  $\langle 0, 1, 1, 0, 1 | a_5^+ a_4 | 0, 1, 1, 1, 0 \rangle$ ,

b.  $\langle 1, 1, 0, 0, 1 | a_1^+ a_3 | 0, 1, 1, 0, 1 \rangle$ ,

c.  $\langle 1, 0, 1, 1, 0 | a_5 a_2 a_4^+ a_3^+ | 1, 1, 0, 0, 1 \rangle$ ,

d.  $\langle 1, 1, 0, 0, 1 | a_1^+ a_3 a_2^+ a_4 | 1, 0, 1, 1, 0 \rangle$ .

**3.5** Using the results of exercises 3.1 - 3.3 prove that for fermions as well, the second quantized form of a general one particle operator  $F^{(1)}$  is:

$$F^{(1)} = \sum_{k,j} f_{kj}^{(1)} a_k^+ a_j.$$

**3.6\*** Prove, that the second quantized form of a general two particle operator  $F^{(2)}$  for fermions is identical to that for bosons!

## 4. Field operators

**4.1** Based on the definition

$$\Psi(\mathbf{r}) = \sum_k a_k \varphi_k(\mathbf{r})$$

$$\Psi^+(\mathbf{r}) = \sum_k a_k^+ \bar{\varphi}_k(\mathbf{r})$$

of the field operators and on the known commutation rules for particle number operators, verify the following commutation relations for field operators:

for bosons:

$$[\Psi(\mathbf{r}), \Psi^+(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'),$$

$$[\Psi(\mathbf{r}), \Psi(\mathbf{r}')] = [\Psi^+(\mathbf{r}), \Psi^+(\mathbf{r}')] = 0;$$

for fermions:

$$\{\Psi(\mathbf{r}), \Psi^+(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}'),$$

$$\{\Psi(\mathbf{r}), \Psi(\mathbf{r}')\} = \{\Psi^+(\mathbf{r}), \Psi^+(\mathbf{r}')\} = 0.$$

**4.2** Prove, that the second quantized form of the one particle operator  $F^{(1)}$  is expressed by field operators as

$$F^{(1)} = \int d^3r \Psi^+(\mathbf{r}) f^{(1)}(\mathbf{r}) \Psi(\mathbf{r}).$$

**4.3** Prove, that the second quantized form of the two particle operator  $F^{(2)}$  is expressed by field operators as

$$F^{(2)} = \int d^3r_1 \int d^3r_2 \Psi^+(\mathbf{r}_1) \Psi^+(\mathbf{r}_2) f^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \Psi(\mathbf{r}_2) \Psi(\mathbf{r}_1).$$

**4.4** With the help of the particle density operator  $\Psi^+(\mathbf{r})\Psi(\mathbf{r})$  and the commutation relations prove, that the state  $\Psi^+(\mathbf{r})|0\rangle$  describes one particle in the point  $\mathbf{r}$  in space. The vacuum state is  $|0\rangle = |N_1 = N_2 = \dots = 0\rangle$ .

**4.5** Determine the second quantized form of the

$$\mathbf{j}(\mathbf{r}) = -e \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \mathbf{v}_i$$

current density operator! The field operator is

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} a_{\mathbf{k}},$$

while the velocity is

$$\mathbf{v}_i = \frac{\mathbf{p}_i + (e/c)\mathbf{A}(\mathbf{r}_i)}{m}.$$

Watch out, the term containing the canonical momentum should be symmetrized!

**4.6** Prove that for a system of identical particles described by the Hamiltonian

$$H = \sum_i [-\hbar^2 \nabla_i^2 / 2m + U(\mathbf{r}_i)],$$

the total particle number operator  $N$  commutes with  $H$ ! Do it simultaneously for fermions and bosons using the sign  $\pm$ .

## 5. Phonons, magnons, bosons

**5.1** The second quantized form of the Hamiltonian of an ionic lattice is

$$H = \sum_{\mathbf{k}, \lambda} \hbar \omega_{\lambda}(\mathbf{k}) \left[ a_{\lambda}^{\dagger}(\mathbf{k}) a_{\lambda}(\mathbf{k}) + \frac{1}{2} \right],$$

where  $\omega_{\lambda}(\mathbf{k})$  is the frequency of the phonon mode  $\lambda$  with wavenumber  $\mathbf{k}$ , while  $a_{\lambda}^{\dagger}(\mathbf{k})$  and  $a_{\lambda}(\mathbf{k})$  creates and annihilates one phonon into or from this mode. If the unit cell contains just a single atom, then the operator of the displacement vector of the ion at lattice point  $\mathbf{R}$  in second quantized form is

$$\mathbf{u}(\mathbf{R}) = \sqrt{\frac{\hbar}{2NM}} \sum_{\mathbf{k}, \lambda} \frac{e^{i\mathbf{k}\mathbf{R}}}{\sqrt{\omega_{\lambda}(\mathbf{k})}} \mathbf{e}_{\lambda}(\mathbf{k}) [a_{\lambda}(\mathbf{k}) + a_{\lambda}^{\dagger}(-\mathbf{k})],$$

where  $M$  is the ionic mass,  $N$  is the number of ions and  $\mathbf{e}_{\lambda}(\mathbf{k})$  is the unit polarization vector of the  $(\lambda, \mathbf{k})$  mode. Suppose, that the gas of phonons is in thermal equilibrium, therefore  $\langle N_{\lambda}(\mathbf{k}) \rangle = \{\exp[\beta \hbar \omega_{\lambda}(\mathbf{k})] - 1\}^{-1}$ .

- a. What is the expectation value of the displacement vector  $\langle \mathbf{u}(\mathbf{R}) \rangle$  of an ion?
- b. What is the expectation value of the square of the displacement vector  $\langle [\mathbf{u}(\mathbf{R})]^2 \rangle$  of an ion?

**5.2** Suppose, that the three acoustic phonon branches in exercise 5.1 are degenerate, and for all  $\lambda = 1, 2, 3$

$$\omega_\lambda(\mathbf{k}) = ck,$$

where  $k < k_D = k_B \Theta_D / \hbar c$ , and  $\Theta_D$  is the Debye temperature. Here  $c$  is the velocity of sound, and the Debye wavenumber  $k_D \approx \pi/a$  is of the order of the inverse lattice spacing.

- a. What is the relative average displacement  $\sqrt{\langle [\mathbf{u}(\mathbf{R})]^2 \rangle} / a$  at low temperatures ( $T \ll \Theta_D$ )?
- b. What is the above ratio for  $T \gg \Theta_D$ ?

**5.3** Suppose that there are  $N$  ions with mass  $M$  each in an ionic lattice with one ion per unit cell. We replace  $N_i (\ll N)$  ions by their isotopes with mass  $M'$ . Due to this replacement, the following perturbation is added to the Hamiltonian of exercise 5.1:

$$H' = \sum_{i=1}^{N_i} \left( \frac{1}{2M'} - \frac{1}{2M} \right) [\mathbf{P}(\mathbf{R}_i)]^2,$$

where  $\mathbf{P}(\mathbf{R})$  is the momentum of the ion at lattice point  $\mathbf{R}$ ,  $\mathbf{R}_i$  is the site of the  $i$ -th isotope, and these sites are random (the probability of each isotopes being at any lattice site is the same).

- a. Using the second quantized form of the momentum operator

$$\mathbf{P}(\mathbf{R}) = \frac{1}{i} \sqrt{\frac{\hbar M}{2N}} \sum_{\mathbf{k}, \lambda} e^{i\mathbf{k}\mathbf{R}} \sqrt{\omega_\lambda(\mathbf{k})} \mathbf{e}_\lambda(\mathbf{k}) [a_\lambda(\mathbf{k}) - a_\lambda^\dagger(-\mathbf{k})]$$

write down  $H'$  in second quantized form, and give the diagrammatic representation of the processes described by each term!

- b. Collect the terms describing scattering of a phonon in  $H'$ , and bring them to the form

$$H'_{scatt} = \sum_{\mathbf{k}, \lambda} \sum_{\mathbf{k}', \lambda'} g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda) a_{\lambda'}^\dagger(\mathbf{k}') a_\lambda(\mathbf{k})$$

(Make use of the commutation rules, and the relations  $\omega_\lambda(-\mathbf{k}) = \omega_\lambda(\mathbf{k})$ , and  $\mathbf{e}_\lambda(-\mathbf{k}) = \mathbf{e}_\lambda(\mathbf{k})$ .) Write down the expression for the  $g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda)$  scattering amplitude!

- c. Based on the form of  $H'_{scatt}$  in point b., express the  $\langle \mathbf{k}', \lambda' | H'_{scatt} | \mathbf{k}, \lambda \rangle$  matrix element with the help of the scattering amplitude  $g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda)$ , then use

Fermi's "golden rule" in order to calculate the  $w(\mathbf{k}, \lambda \rightarrow \mathbf{k}', \lambda')$  transition probability per unit time! (Here, except for the states  $(\lambda, \mathbf{k})$  and  $(\lambda', \mathbf{k}')$ , the number of phonons in other modes do not change.)

- d. The change of the number of phonons per unit time in the mode  $(\lambda, \mathbf{k})$  due to scattering out of this mode is:

$$\frac{\partial}{\partial t} N_\lambda(\mathbf{k})|_{out} = - \sum_{\mathbf{k}', \lambda'} w(\mathbf{k}, \lambda \rightarrow \mathbf{k}', \lambda').$$

On the other hand phenomenologically

$$\frac{\partial}{\partial t} N_\lambda(\mathbf{k})|_{out} = - \frac{N_\lambda(\mathbf{k})}{\tau_\lambda(\mathbf{k})}.$$

Express the  $1/\tau_\lambda(\mathbf{k})$  inverse lifetime of the  $(\lambda, \mathbf{k})$  phonon with the help of  $g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda)$ !

- e. Utilizing the result for  $g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda)$  obtained in point b., calculate the quantity  $|g(\mathbf{k}', \lambda'; \mathbf{k}, \lambda)|^2$  averaged over the random positions of the isotopes. Use the following definition of the average:

$$\bar{f}(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{N_i}) = \frac{1}{N} \sum_{\mathbf{R}_1} \frac{1}{N} \sum_{\mathbf{R}_2} \dots \frac{1}{N} \sum_{\mathbf{R}_{N_i}} f(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{N_i}).$$

- f. Calculate  $1/\tau_\lambda(\mathbf{k})$  (see point d.) based on the result obtained in point e.! (Utilize that in thermal equilibrium  $N_\lambda(\mathbf{k}) = \{\exp[\beta\hbar\omega_\lambda(\mathbf{k})] - 1\}^{-1}$ .)
- g. Suppose that all acoustic branches are degenerate, therefore  $\omega_\lambda(\mathbf{k}) = ck$  for all  $\lambda = 1, 2, 3$ , where  $c$  is the velocity of sound. Then for each wavenumber  $\mathbf{k}$  the system of unit polarization vectors  $\mathbf{e}_\lambda(\mathbf{k})$  can be directed arbitrarily (as long as they are mutually orthogonal). For example even  $\mathbf{e}_\lambda(\mathbf{k}') = \mathbf{e}_\lambda(\mathbf{k})$  can be chosen for each  $\mathbf{k}'$ . Exploiting this, calculate  $1/\tau_\lambda(\mathbf{k})$  at zero temperature! How does  $1/\tau(\mathbf{k})$  depend on  $\mathbf{k}$ ?
- h. Evaluate the relative damping  $1/\omega(\mathbf{k})\tau(\mathbf{k})$  also at zero temperature!

**5.4** The spin operators can be expressed with the  $a, a^+$  bose operators ( $aa^+ - a^+a = 1$ ):

$$S^+ = \sqrt{2S}a^+(1 - \frac{a^+a}{2S}),$$

$$S^- = \sqrt{2S}a,$$

and

$$S^z = a^+a - S.$$



- a. Show that with such a definition the spin operators satisfy the spin commutation relations:  $[S^+, S^-] = 2S^z$ ,  $[S^-, S^z] = S^-$ ,  $[S^z, S^+] = S^+$ .

- b. Express the

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

Heisenberg Hamiltonian with the bose operators!  $\langle i, j \rangle$  means nearest neighbors.

- c. Retaining terms with two operators only, diagonalize  $H$  with the following transformation:

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_i} a_{\mathbf{q}}.$$

Let the spins reside on a cubic lattice with lattice constant  $b$ . How does the energy spectrum behave for small wavenumbers?

- d. Calculate the low temperature specific heat!

### 5.5 The Hamiltonian of bosons scattered by impurities is

$$H = \sum_{a=1}^N -\frac{\hbar^2 \nabla_a^2}{2m} + \sum_{a=1}^N \sum_{j=1}^{N_i} V_0 \delta(r_a - R_j),$$

where the second term can be considered as perturbation (the number of impurities is  $N_i \ll N$ ).

- a. Calculate the second quantized form of the above operators with the help of the following field operator:

$$\Psi(r) = \sum_k \frac{1}{\sqrt{V}} e^{ikr} a_k!$$

- b. Determine the transition probability per unit time  $w(\mathbf{k} \rightarrow \mathbf{k}')$  due to the impurity scattering, with the help of Fermi's golden rule!
- c. Determine the inverse lifetime, then calculate its average due to the random position of the impurities!

### 5.6 Consider the following Hamiltonian:

$$H = \int_{-L/2}^{L/2} \frac{v}{2} \left[ \Pi^2(x) + \left( \frac{\partial \phi(x)}{\partial x} \right)^2 \right] dx,$$

where the  $\Pi$  and  $\phi$  fields obey canonical commutation relations:  $[\Pi(x), \phi(x')] = -i\delta(x - x')$ . Using the above equations derive the equations of motion for the fields  $\Pi$  and  $\phi$ ! Show that these satisfy a wave equation, and  $v$  is just the velocity of the wave.

**5.7** The density-density correlation function of the ideal gas of free noninteracting spinless bosons is given by

$$\langle n(\mathbf{r}_1)n(\mathbf{r}_2) \rangle = n^2\nu(\mathbf{r}_1, \mathbf{r}_2) + n\delta(\mathbf{r}_1 - \mathbf{r}_2) + n^2$$

in thermal equilibrium, with  $n = N/V$  being the density of the gas and with  $n(\mathbf{r})$  being the operator of the particle density. Calculate the function  $\nu$  in the following steps:

- Write down the field operator of the bose gas on the one particle basis which fits best for the problem, then give the second quantized form of the Hamiltonian  $H$  of the system and that of the operator  $H - \mu N$ !
- Write down the second quantized form of the particle density operator, then using this result calculate the thermodynamic expectation value  $\langle n(\mathbf{r}_1)n(\mathbf{r}_2) \rangle$ , and the resulting  $\nu(\mathbf{r}_1, \mathbf{r}_2)$  function! Show that  $\nu(\mathbf{r}_1, \mathbf{r}_2)$  depends only on the difference of its arguments! (Guidance: according to Wick's theorem  $\langle a_i^+ a_j a_k^+ a_l \rangle = \langle a_i^+ a_j \rangle \langle a_k^+ a_l \rangle + \langle a_i^+ a_l \rangle \langle a_j a_k^+ \rangle$ .)

## 6. Electrons I.

**6.1** The Hamiltonian of a spin  $S = 1/2$  interacting fermi system is:

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j).$$

The wavefunction of the  $(\mathbf{k}, \sigma)$  one particle eigenstate is

$$\varphi_{\mathbf{k}, \sigma}(\mathbf{r}, \beta) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}} \delta_{\sigma\beta},$$

where  $\sigma, \beta = \uparrow, \downarrow$ , and these wavefunctions form an orthonormal system:

$$\sum_{\beta} \int d^3r \bar{\varphi}_{\mathbf{k}, \sigma}(\mathbf{r}, \beta) \varphi_{\mathbf{k}', \sigma'}(\mathbf{r}, \beta) = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}.$$

Prove that the second quantized form of  $H$  is

$$H = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k},\sigma}^+ a_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\sigma,\sigma'} \tilde{V}(\mathbf{q}) a_{\mathbf{k}+\mathbf{q},\sigma}^+ a_{\mathbf{k}'-\mathbf{q},\sigma'}^+ a_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma},$$

where

$$\tilde{V}(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\mathbf{r}} V(\mathbf{r})$$

is the Fourier transformed pair interaction.

- 6.2** Prove that the expectation value of the Hamiltonian of exercise 6.1 in the many body state characterized by the set of occupation numbers  $\{n_{\mathbf{k},\sigma}\}$  (often called the distribution function) is ( $\sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma} = N = \text{const.}$ ):

$$\begin{aligned} E\{n_{\mathbf{k},\sigma}\} &= \langle \{n_{\mathbf{k},\sigma}\} | H | \{n_{\mathbf{k},\sigma}\} \rangle = \\ &= \sum_{\mathbf{k},\sigma} \frac{\hbar^2 k^2}{2m} n_{\mathbf{k},\sigma} - \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}',\sigma} \tilde{V}(\mathbf{k} - \mathbf{k}') n_{\mathbf{k},\sigma} n_{\mathbf{k}',\sigma}, \end{aligned}$$

if we disregard a constant independent of the  $\{n_{\mathbf{k},\sigma}\}$  distribution.

- 6.3** The result of exercise 6.2 yields the total energy of interacting electrons up to first order in the perturbation series with respect to the interaction, where we kept only the exchange term omitting the structureless direct term.

- a. In the spirit of Fermi liquid theory the one particle spectrum can be calculated from the change in total energy due to the change in the occupation numbers:

$$\delta E = \sum_{\mathbf{k},\sigma} \varepsilon_{\sigma}(\mathbf{k}) \delta n_{\mathbf{k},\sigma},$$

where  $\varepsilon_{\sigma}(\mathbf{k})$  depends on the set  $\{n_{\mathbf{k},\sigma}\}$  in general. Prove that the quasiparticle spectrum is

$$\varepsilon_{\sigma}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} - \frac{1}{V} \sum_{\mathbf{k}'} \tilde{V}(\mathbf{k} - \mathbf{k}') n_{\mathbf{k}',\sigma}.$$

(Utilize that  $\tilde{V}(-\mathbf{q}) = \tilde{V}(\mathbf{q})$  if  $V(-\mathbf{r}) = V(\mathbf{r})$ .)

- b. By definition, the velocity of the quasiparticles is

$$\mathbf{v}_{\sigma}(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} \varepsilon_{\sigma}(\mathbf{k}).$$

Prove that

$$\mathbf{v}_{\sigma}(\mathbf{k}) = \frac{\hbar}{m} \mathbf{k} - \frac{1}{\hbar} \int \frac{d^3k'}{(2\pi)^3} \tilde{V}(\mathbf{k} - \mathbf{k}') \frac{\partial}{\partial \mathbf{k}'} n_{\mathbf{k}',\sigma}.$$

(Utilize that  $\frac{1}{V} \sum_{\mathbf{k}} \rightarrow \int \frac{d^3k}{(2\pi)^3}$ , and perform partial integration.)

- c. At zero temperature  $n_{\mathbf{k},\sigma} = 1$ , if  $k < k_F$ , and  $n_{\mathbf{k},\sigma} = 0$ , if  $k > k_F$ , therefore

$$\frac{\partial}{\partial \mathbf{k}} n_{\mathbf{k},\sigma} = -\delta(k - k_F) \frac{\mathbf{k}}{k}.$$

If the interaction is spherically symmetric, i.e.  $\tilde{V}(\mathbf{k} - \mathbf{k}') = \tilde{V}(|\mathbf{k} - \mathbf{k}'|)$ , then the velocity can be brought to the form  $\mathbf{v}(\mathbf{k}) = \hbar \mathbf{k} / m^*$ , where  $m^*$  depends only on the length of  $\mathbf{k}$ . Prove that on the Fermi surface (for  $k = k_F$ )

$$\frac{1}{m^*} = \frac{1}{m} + \frac{k_F}{(2\pi)^3 \hbar^2} \int d\Omega \hat{V}(\vartheta) \cos \vartheta,$$

where  $\hat{V}(\vartheta) = \tilde{V}[2k_F \sin(\vartheta/2)]$ .

- 6.4** Suppose that the interaction in exercise 6.3 is the unscreened Coulomb interaction:

$$\tilde{V}(\mathbf{q}) = \frac{4\pi e^2}{q^2}.$$

- a. Prove that the quasiparticle excitation spectrum at zero temperature is

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} F(k/k_F),$$

where

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|.$$

Sketch the function  $F(x)$ !

- b. Prove that the ground state energy per unit volume is

$$\frac{E}{V} = \frac{\hbar^2 k_F^5}{10\pi^2 m} - \frac{e^2 k_F^4}{4\pi^3}.$$

- c. Calculate the ground state energy per particle  $E/N$ ! (Use the relation between the particle density  $N/V$  and the Fermi wavenumber  $k_F$ .)
- d. The natural unit of atomic energies is the Rydberg.  $1\text{Ry} = e^2/2a_0 (= 13.6\text{eV})$ , where  $a_0 = \hbar^2/m_e^2 (= 0.529\text{\AA})$  is the Bohr radius. Express the result of point c. in Ry! (The result depends only on the value of  $a_0 k_F$ .)
- e. The radius  $r_s$  defined by

$$\frac{V}{N} = \frac{4\pi}{3} r_s^3$$

characterizes the average distance of the particles. What is the relation between  $k_F$  and  $r_s$ ? Write down the result of point d. as a function of  $a_0$  and  $r_s$ ! Evaluate the numerical coefficients!

**6.5** We have seen in exercise 6.4 that the ground state energy per particle of the interacting electron gas is

$$\frac{E}{N} = \left[ 2.21 \left( \frac{a_0}{r_s} \right)^2 - 0.916 \frac{a_0}{r_s} \right] \text{Ry},$$

where  $a_0$  is the Bohr radius, while  $r_s$  is the radius of a sphere, the volume of which is equal to the system volume per electron number. The first term is the kinetic energy and the second is the Coulomb exchange energy, i.e. the first order correction from the perturbation series with respect to the interaction. Obviously, this expression is reliable only if the correction is relatively small, i. e. if  $a_0/r_s$  is large, in other words for dense electron gas. In case of a dilute electron gas (large  $r_s/a_0$ ) the interaction term dominates, and therefore the nature of the ground state changes radically, the electrons may order themselves into a regular crystal lattice (Wigner crystal). Calculate the energy of the Wigner crystal in the following steps:

- Suppose that any single electron of the system is allowed to move within a sphere of radius  $r_s$  around its lattice point, and the compensating charge of the ions is uniformly distributed within the sphere. Prove that if the electron is located at a distance  $r$  from the center of the sphere, then the potential energy of the system has the form

$$V(\mathbf{r}) = \alpha + \beta r^2.$$

Evaluate the constants  $\alpha$  and  $\beta$ ! (Do not forget about the energy of the charged sphere either!)

- Supplementing the above potential energy with the kinetic energy of the electron, the full Hamiltonian reads as

$$H = \frac{p^2}{2m} + \beta r^2 + \alpha,$$

which defines a harmonic oscillator with respect to the electron. Calculate the frequency  $\omega$  of this oscillator using the result for  $\beta$  obtained in point a.!

- Clearly, the ground state energy per electron of the Wigner crystal is given by the ground state energy of the Hamiltonian in point b. How much is this energy? (Do not forget, that there is a three dimensional oscillator in point b.!) Express this energy in Ry with the help of  $a_0/r_s$ !
- The expectation value of the squared amplitude of a harmonic oscillator in its ground state is

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega}.$$

How much is the relative expectation value  $\sqrt{\langle r^2 \rangle}/r_s$  of the distance of the electron from its equilibrium position? Express the result with the help of  $a_0/r_s$ !

**6.6** Let  $h^{at}$  be the spin independent Hamiltonian of an idealized two level atom:

$$h^{at}\varphi_\alpha(\mathbf{r}) = \varepsilon_\alpha\varphi_\alpha(\mathbf{r}),$$

where  $\alpha = 1, 2$ . We turn on a homogeneous electric field  $\mathbf{E}$  parallel to the  $z$  direction, in order to polarize the atom. The interaction of a single electron with the field is described by  $h' = -\mathbf{E}\mathbf{d}$ , where  $\mathbf{d} = -e\mathbf{r}$  is the dipole vector of the electron. Write down the field operator for the electron, then give the second quantized form of the full Hamilton operator  $H$  of the noninteracting atomic electron system (do not forget about the spin). Is the atom polarizable, if the states  $\varphi_\alpha$  have spherical symmetry?

## 7. Electrons II.

**7.1** The Hamiltonian of the one band Hubbard model in Wannier representation is

$$H = t \sum_{\mathbf{R}, \mathbf{d}, \sigma} a_{\mathbf{R}, \sigma}^\dagger a_{\mathbf{R}+\mathbf{d}, \sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}, \uparrow} n_{\mathbf{R}, \downarrow}.$$

Introduce the following linear combinations of the Wannier operators:

$$a_{\mathbf{k}, \sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} a_{\mathbf{R}, \sigma}.$$

a. Prove that the inverse (Bloch  $\rightarrow$  Wannier) transformation has the form

$$a_{\mathbf{R}, \sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} a_{\mathbf{k}, \sigma}.$$

b. The kinetic energy term of  $H$  can be diagonalized by the above transformation as:

$$H^{kin} = \sum_{\mathbf{k}, \sigma} \varepsilon(\mathbf{k}) a_{\mathbf{k}, \sigma}^\dagger a_{\mathbf{k}, \sigma}.$$

Determine  $\varepsilon(\mathbf{k})$ !

- c. Perform the above transformation on the interaction term of  $H$  as well! Comparing this with the result of exercise 6.1, what difference can be seen?

**7.2** Show that considering electron-phonon scattering there will be Umklapp processes, meaning that the change in the wavenumber of the electron is equal to the wavenumber of the phonon only up to a reciprocal lattice vector! Guidance: the second quantized form of the operator  $e^{i\mathbf{q}\mathbf{r}}$  should be obtained, the wavefunction of the electron, according to the Bloch theorem is  $\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$ , where  $u_{\mathbf{k}}(\mathbf{r})$  is lattice periodic.

**7.3** Show that, similar to electron-phonon scattering, there are Umklapp processes considering electron-electron scattering as well, during which the total wavenumber is conserved only up to a reciprocal lattice vector! Guidance: according to the Bloch-theorem  $\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$ , where  $u_{\mathbf{k}}(\mathbf{r})$  is lattice periodic, and can be expanded in Fourier series.

**7.4** In the unit cell of a one dimensional lattice there are two atoms (with a single energy level each). The energies of the levels are  $\varepsilon_1$  and  $\varepsilon_2$ , the values of the two nearest neighbor hopping integrals are  $t_1$  and  $t_2$  (both real). The second quantized form of the Hamiltonian of this system (without interaction) in Wannier representation is

$$\begin{aligned} H^{kin} = & \varepsilon_1 \sum_{\mathbf{R},\sigma} a_{1,\mathbf{R},\sigma}^+ a_{1,\mathbf{R},\sigma} + \varepsilon_2 \sum_{\mathbf{R},\sigma} a_{2,\mathbf{R},\sigma}^+ a_{2,\mathbf{R},\sigma} + \\ & + t_1 \sum_{\mathbf{R},\sigma} (a_{1,\mathbf{R},\sigma}^+ a_{2,\mathbf{R},\sigma} + a_{2,\mathbf{R},\sigma}^+ a_{1,\mathbf{R},\sigma}) + \\ & + t_2 \sum_{\mathbf{R},\sigma} (a_{1,\mathbf{R},\sigma}^+ a_{2,\mathbf{R}-\mathbf{a},\sigma} + a_{2,\mathbf{R}-\mathbf{a},\sigma}^+ a_{1,\mathbf{R},\sigma}), \end{aligned}$$

where  $\mathbf{a}$  is the unit translation vector. Using the usual transformation ( $i = 1, 2$ )

$$a_{i,\mathbf{R},\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} a_{i,\mathbf{k},\sigma},$$

$H^{kin}$  can be brought to the following form:

$$H^{kin} = \sum_{\mathbf{k},\sigma} \sum_{i,j} a_{i,\mathbf{k},\sigma}^+ h_{ij}(\mathbf{k}) a_{j,\mathbf{k},\sigma},$$

where the different  $\mathbf{k}$  values have already decoupled, but the operator is not yet fully diagonalized.

- Calculate the matrix elements  $h_{ij}(\mathbf{k})$  ( $i, j = 1, 2$ )!
- The dispersion relation of the two band model is given by the eigenvalues  $E_{\pm}(\mathbf{k})$  of the  $2 \times 2$  matrix  $\{h_{ij}(\mathbf{k})\}$ . Determine the  $E_{\pm}(\mathbf{k})$  band structure!

- c. Supposing that  $t_1$  and  $t_2$  have the same sign, how big is the gap in the spectrum?
- d. Sketch the band structure ( $E_{\pm}(\mathbf{k})$ ) for  $\varepsilon_1 = \varepsilon_2 = 0$ ,  $t_1 = t_2 = t$ !

**7.5** The most important part of the high temperature superconductors is the  $\text{CuO}_2$  plane, in which the copper atoms form a square lattice with lattice constant  $a$ , while the oxygen atoms are sitting at the middle of the line segments connecting nearest neighbor copper atoms. The simplest model takes into account the hopping integrals between the copper and its neighboring oxygens only. Due to symmetry reasons and to the properties of the atomic orbitals participating in the hybridization (copper  $d$  and oxygen  $p$  orbitals) the hopping integral between the copper and the oxygens located in the positive  $\mathbf{x}$  and  $\mathbf{y}$  direction from the copper is  $t$ , while it is  $-t$  towards the oxygens located in the negative  $\mathbf{x}$  and  $\mathbf{y}$  direction from the copper.

- a. Sketch the structure of the  $\text{CuO}_2$  plane, identify the unit cell and the nearest neighbor hopping integrals!
- b. Let the site energy on the copper be  $\varepsilon$ , while that on the oxygen be 0. Write down the Hamiltonian (self adjoint!) of the system in Wannier representation, if  $a_{i,\mathbf{R},\sigma}^+$  and  $a_{i,\mathbf{R},\sigma}$  creates and annihilates an electron in unit cell  $\mathbf{R}$  on the  $i$ -th atom ( $i = 1, 2, 3$ )! Use the formalism developed in the previous exercise!
- c. Applying the following transformation

$$a_{i,\mathbf{R},\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} a_{i,\mathbf{k},\sigma}$$

the Hamiltonian can be brought to the following form:

$$H = \sum_{\mathbf{k},\sigma} \sum_{i,j} a_{i,\mathbf{k},\sigma}^+ h_{ij}(\mathbf{k}) a_{j,\mathbf{k},\sigma}.$$

Give the matrix elements  $h_{ij}(\mathbf{k})$ !

- d. The model's dispersion is given by the eigenvalues of the  $3 \times 3$  matrix  $\{h_{ij}(\mathbf{k})\}$ . Determine the band structure!

**7.6** The magnetization (for small magnetic fields) of the Hubbard model is given by

$$\langle M_z \rangle = V \chi_0 H_{eff}$$

in mean field approximation, where

$$\chi_0 = \mu_B^2 \frac{2}{V} \sum_{\mathbf{k}} \{-f'[\varepsilon(\mathbf{k}) - \mu]\}$$



is the susceptibility of the noninteracting system, and

$$H_{eff} = H + \frac{U \langle M_z \rangle}{2N \mu_B^2}$$

is the effective field. Then the magnetization can be brought to the form

$$\langle M_z \rangle = V \chi H,$$

which defines the susceptibility  $\chi$  of the interacting system in mean field approximation. Suppose that the hopping integral  $t \rightarrow 0$ , i.e. it is getting difficult for the electrons to move. The band gets narrow, and the density of states

$$g(\varepsilon) = \frac{2}{V} \sum_{\mathbf{k}} \delta[\varepsilon - \varepsilon(\mathbf{k})] \rightarrow \frac{2}{V_c} \delta(\varepsilon).$$

Then at finite temperatures the derivative of the Fermi function in the expression for  $\chi_0$  can obviously not be approximated by the Dirac delta function.

- Calculate the noninteracting susceptibility  $\chi_0$  for this narrow band case! Give the result as a function of  $n = N_e/N$ , the average electron number per lattice site!
- According to the theory of atomic paramagnetism, the Curie susceptibility of  $S = 1/2$  spins *localized* on lattice sites is:

$$\chi_0^{Curie} = \frac{\mu_B^2}{V_c} \frac{1}{k_B T}.$$

How much is the susceptibility  $\chi_0$  calculated in point a. in the corresponding  $n = 1$  case (half filled band)? What could be the explanation for the difference between  $\chi_0$  determined in such a way and  $\chi_0^{Curie}$ ? If the question is too difficult, continue with point c.

- Calculate the susceptibility  $\chi$  of the interacting ( $U \neq 0$ ) system in mean field approximation for arbitrary  $n$ ! Does the expression for  $\chi$  indicate phase transition at finite temperatures? If yes, what is the critical temperature  $T_c$ ? What are  $\chi$  and  $T_c$  for a half filled band?

**7.7** The problem in exercise 7.6 ( $t \rightarrow 0$  Hubbard modell) is exactly solvable, since the individual lattice sites decouple completely. This is a good occasion to demonstrate the limits of the mean field approximation.

- First prove that the magnetic term

$$H_{Zeeman} = \mu_B H \sum_{\mathbf{k}, \sigma} \sigma a_{\mathbf{k}, \sigma}^{\dagger} a_{\mathbf{k}, \sigma}$$

is expressed with the  $a_{\mathbf{R},\sigma}^+$  and  $a_{\mathbf{R},\sigma}$  Wannier operators as

$$H_{Zeeman} = \mu_B H \sum_{\mathbf{R},\sigma} \sigma a_{\mathbf{R},\sigma}^+ a_{\mathbf{R},\sigma}.$$

(Utilize the Fourier transformation encountered in exercise 7.1)

b. Then clearly, the full Hamiltonian is

$$H(t \rightarrow 0) = \sum_{\mathbf{R}} H(\mathbf{R}),$$

where

$$H(\mathbf{R}) = \mu_B H (n_{\mathbf{R},\uparrow} - n_{\mathbf{R},\downarrow}) + U n_{\mathbf{R},\uparrow} n_{\mathbf{R},\downarrow}$$

depends only on the occupation numbers of a single lattice site only. The grand canonical partition function of the full system is  $\Xi = \Theta^N$ , where  $\Theta$  is the grand canonical partition function of a single site. The following states are possible on a single lattice site:

0 electron ( $n_{\mathbf{R},\uparrow} = n_{\mathbf{R},\downarrow} = 0$ )

1 electron in the state  $\uparrow$  ( $n_{\mathbf{R},\uparrow} = 1; n_{\mathbf{R},\downarrow} = 0$ )

1 electron in the state  $\downarrow$  ( $n_{\mathbf{R},\uparrow} = 0; n_{\mathbf{R},\downarrow} = 1$ )

2 electrons ( $n_{\mathbf{R},\uparrow} = n_{\mathbf{R},\downarrow} = 1$ )

How much is the energy  $E$  of these states? Write down the partition function  $\Theta$ ! (Let the chemical potential be  $\mu$ , and use the expression  $\Theta = \sum e^{-\beta(E-\mu N)}$  where  $N$  is now the number of particles on the given site in the given state.)

c. The grand canonical thermodynamic potential of the full system is

$$\Omega = -\frac{1}{\beta} \ln \Xi = -\frac{N}{\beta} \ln \Theta.$$

The number of electrons is  $N_e = -\partial\Omega/\partial\mu$ , while the magnetization of the system is  $M_z = -\partial\Omega/\partial H$ . Using the results of point b. determine the quantities  $n = N_e/N$  and  $m = M_z/N$  as a function of  $\mu$  and  $H$ !

d. What is the susceptibility

$$\chi = \frac{1}{V} \frac{\partial M_z}{\partial H}$$

of the system in the limit  $H \rightarrow 0$  as a function of  $\mu$ ?

e. Using the result obtained in point c. express the chemical potential  $\mu$  with the help of  $n$ , in the limit  $H \rightarrow 0$ ! What is  $\mu$  for a half filled band ( $n = 1$ )?

- f. What is the susceptibility determined in point d. for  $n = 1$ ? Does this exact result indicate a phase transition at some finite temperature? Expand the inverse of the exact susceptibility in powers of  $U$ ! What do you experience by comparing this with the mean field result of point 7.6.c? What is the exact susceptibility for  $U \gg k_B T$ ? Compare this with the Curie susceptibility of point 7.6.b! Is the answer to the last question of point 7.6.b any easier now?

**7.8** The half filled Hubbard model is described by the following Hamiltonian:

$$H = -t \sum_{i,\sigma} (c_{i,\sigma}^+ c_{i+1,\sigma} + h.c.) + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}).$$

Let's define the following operators:

$$J^z = \frac{1}{2} \sum_i (c_{i\uparrow}^+ c_{i\uparrow} + c_{i\downarrow}^+ c_{i\downarrow} - 1), \quad J^+ = \sum_i (-1)^i c_{i\downarrow}^+ c_{i\uparrow}, \quad J^- = \sum_i (-1)^i c_{i\uparrow} c_{i\downarrow}.$$

- Prove that these operators satisfy the usual  $SU(2)$  commutation relations!
- Is the operator  $\mathbf{J}$  a conserved quantity?

## 8. Condensates

**8.1** In case of a spin density wave in mean field approximation the Hamiltonian can be diagonalized by the quasiparticle operators

$$d_{+,k,\sigma} = \sigma e^{-i\varphi} u_k a_{k,\sigma} + v_k a_{k-2k_F,\sigma}$$

$$d_{-,k,\sigma} = \sigma e^{-i\varphi} v_k a_{k,\sigma} - u_k a_{k-2k_F,\sigma}$$

to obtain the following expression:

$$H = \sum_{\alpha,k,\sigma} \alpha \sqrt{\xi_k^2 + |\Delta|^2} d_{\alpha,k,\sigma}^+ d_{\alpha,k,\sigma}.$$

Here

$$u_k = \sqrt{\frac{1}{2} \left[ 1 + \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta|^2}} \right]},$$

$v_k = \sqrt{1 - u_k^2}$ ,  $\alpha = \pm$ , and  $k$  takes values from the reduced Brillouin zone corresponding to the new periodicity. The ground state of the system can be described by

$$|\psi_0\rangle = \prod_{k,\sigma} d_{-,k,\sigma}^+ |0\rangle,$$

and the ground state energy  $E_0 = \langle \psi_0 | H | \psi_0 \rangle$  is independent of the phase  $\varphi$  of the spin density wave. Consider a state, which is obtained from the ground state in such a way, that we change the phase relations of one quasiparticle  $(-, k_0, \sigma_0)$ :

$$|\psi\rangle = [\sigma_0 e^{-i(\varphi+\delta\varphi)} v_{k_0} a_{k_0, \sigma_0} - u_{k_0} a_{k_0-2k_F, \sigma_0}]^+ \prod_{(k, \sigma) \neq (k_0, \sigma_0)} d_{-, k, \sigma}^+ |0\rangle.$$

Prove that the energy expectation value of this state exceeds  $E_0$  by the following amount:

$$\delta E = \frac{|\Delta|^2}{\sqrt{\xi_{k_0}^2 + |\Delta|^2}} [1 - \cos(\delta\varphi)].$$

**8.2** The one band Hubbard model for spinless bosons is

$$H = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{U}{2} \sum_{\mathbf{R}} n_{\mathbf{R}} (n_{\mathbf{R}} - 1),$$

where  $n_{\mathbf{R}} = a_{\mathbf{R}}^+ a_{\mathbf{R}}$ , and the relation between operators acting in real and momentum space has the usual form:

$$a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} a_{\mathbf{R}}$$

( $N$  is the number of lattice points). The ground state of noninteracting ( $U = 0$ ) bosons is the Bose condensed state

$$|\psi_0\rangle = \frac{1}{\sqrt{N_B!}} (a_{\mathbf{k}=0}^+)^{N_B} |0\rangle,$$

where  $|0\rangle$  is the vacuum state,  $N_B$  is the number of bosons, and each boson is in the state  $\mathbf{k} = 0$ . Since  $a_{\mathbf{k}=0} = (1/\sqrt{N}) \sum_{\mathbf{R}} a_{\mathbf{R}}$ , therefore the real space structure of this ground state is

$$|\psi_0\rangle = \frac{1}{\sqrt{N_B!}} \frac{1}{\sqrt{N}^{N_B}} \sum_{\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{N_B}} a_{\mathbf{R}_1}^+ a_{\mathbf{R}_2}^+ \dots a_{\mathbf{R}_{N_B}}^+ |0\rangle.$$

Following Gutzwiller we can imagine the ground state of the strongly interacting ( $U \rightarrow \infty$ ) system in such a way, that we omit those states from the above linear combination, which contains two (or more) bosons on the same lattice site. (Then clearly  $N_B \leq N$  has to be satisfied.) The trial wavefunction obtained in such a way (by projection) is:

$$|P\psi_0\rangle = \frac{1}{\sqrt{N_B!}} \frac{1}{\sqrt{N}^{N_B}} \sum_{\mathbf{R}_1 \neq \mathbf{R}_2 \neq \dots \neq \mathbf{R}_{N_B}} a_{\mathbf{R}_1}^+ a_{\mathbf{R}_2}^+ \dots a_{\mathbf{R}_{N_B}}^+ |0\rangle.$$

Prove that in this state the expectation value of the occupation number of the  $\mathbf{k} = 0$  one particle state  $n_{\mathbf{k}=0} = a_{\mathbf{k}=0}^\dagger a_{\mathbf{k}=0}$  given by

$$\langle n_{\mathbf{k}=0} \rangle = \frac{\langle P\psi_0 | n_{\mathbf{k}=0} | P\psi_0 \rangle}{\langle P\psi_0 | P\psi_0 \rangle}$$

is evaluated as:

$$\langle n_{\mathbf{k}=0} \rangle = N_B \left[ 1 - \frac{N_B - 1}{N} \right],$$

i.e. it is the total number of bosons reduced by a factor depending on the density of bosons.