

## Theory of collective oscillations in strongly correlated electron systems

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1994 J. Phys.: Condens. Matter 6 2225

(<http://iopscience.iop.org/0953-8984/6/11/011>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.147

The article was downloaded on 12/05/2010 at 17:56

Please note that [terms and conditions apply](#).

# Theory of collective oscillations in strongly correlated electron systems

Sergey S Moliver

M V Lomonosov Moscow State University Branch 42, L N Tolstoy Street, Ulyanovsk.  
432 700 Russia

Received 7 May 1993, in final form 25 August 1993

**Abstract.** A dispersion relation is derived for the collective oscillation mode in a strongly correlated electron system, described by a single-band lattice Hubbard model. On the basis of the equations of motion for a pair of propagators (one- and two-electron causal temperature Green functions), a self-oscillatory condition is formulated and obtained by the same technique as the superconductor susceptibility to a variable external field. The equations of motion are subdivided into a stationary part and an oscillatory part. The stationary part establishes a self-consistent relation between the chemical potential and the occupancy numbers of the thermodynamic equilibrium state, and it can be applied to any variously ordered *a priori* ground state. The oscillatory part yields a dispersion relation for the collective oscillation mode, and it is considered for a system with translationally invariant ground state.

## 1. Introduction

The aim of this work is to present a theoretical method for the calculation of the dispersion relation between frequency and wavevector of a collective boson-type oscillation mode in a strongly correlated electron system. We denote this relation by  $\omega_{\text{cor}}(\mathbf{q})$  and call this collective mode a *correlation oscillation* to distinguish it from a *plasmon* oscillation (Moliver 1989, 1991).

When dealing with collective electron phenomena, the theory of  $\omega_{\text{cor}}(\mathbf{q})$  should be compared with the well known plasmon one. Essential differences between the two types of oscillations—correlation and plasmon—may be seen from the following. Plasmons can be excited in any system of charged particles owing to the long-range Coulomb interaction between a particle in site  $j$  and the macroscopic charge density near site  $i$ :

$$H_{\text{int}} = \sum_{\substack{i,j \\ \sigma,\sigma'}} \frac{e^2 \langle n_{i\sigma} \rangle n_{j\sigma'}}{|\mathbf{r}_{ij}|} \quad (1)$$

The fingerprint of a strongly correlated system is the short-range electron–electron interaction of the Hubbard form

$$H_{\text{cor}} = U \sum_i n_{i\sigma} n_{i,-\sigma} \quad n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \quad (2)$$

where creation operator  $c^\dagger$  and occupancy operator  $n$  are written in the basis of site ( $i$ ) and spin ( $\sigma$ ) wavefunctions. While interaction (1) may be treated by perturbation theory,

interaction (2) cannot be taken as a perturbation in a strongly correlated system; rather it must be held in the unperturbed Hamiltonian.

Since the problem of the ground state of a strongly correlated system is as yet unsolved, we would not like to mix it with the present theory of  $\omega_{\text{cor}}(\mathbf{q})$ ; so, we assume the averages  $\langle c_{m,\pm\sigma}^\dagger c_{i\sigma} \rangle$  of the grand canonical ensemble (with temperature  $T$  and chemical potential  $\mu$ ) as *a priori* parameters. As an advantage, our method can be applied to variously ordered ground states, giving new opportunities to the experimental studies of ordering in strongly correlated systems.

## 2. Temperature Green functions equations of motion

We consider a simple single-band Hubbard lattice model in order to achieve analytical final equations for  $\omega_{\text{cor}}(\mathbf{q})$ . In the several-band case some steps (see section 4) can be made numerically, but the final result is also achievable in the form of a computational procedure. Besides (2), the single-band model includes (Doniach and Sondheimer 1974)

$$H_{\text{band}} = \sum_{i,\sigma} (\varepsilon_0 - \mu) n_{i\sigma} + \sum_{i \neq j, \sigma} t(\mathbf{r}_{ij}) c_{i\sigma}^\dagger c_{j\sigma}. \quad (3)$$

The one-electron effective lattice potential (or the so-called hopping integral) has either a site ( $ij$ ) or a wavevector  $\mathbf{k}$  representation ( $\mathbf{k}$  belongs to the Brillouin zone)

$$t(\mathbf{r}_{ij}) = \frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} \exp(-i\mathbf{k}\mathbf{r}_{ij}). \quad (4)$$

In order to have a ground-state-independent temperature method, we proceed with the temperature-ordered (causal) Green functions (Abrikosov *et al* 1963)

$$G_{ij}^\pm(\tau, \tau') = -\langle T_\tau c_{i\sigma}(\tau) c_{j,\pm\sigma}^\dagger(\tau') \rangle \quad (5a)$$

$$\Delta_{ij}^\pm(\tau, \tau') = -\langle T_\tau n_{i,-\sigma}(\tau) c_{i\sigma}(\tau) c_{j,\pm\sigma}^\dagger(\tau') \rangle \quad (5b)$$

where  $\tau$  is an 'imaginary time' variable in the Heisenberg representation of operators

$$c(\tau) = e^{H\tau} c e^{-H\tau} \quad 0 < \tau < T^{-1} \quad (6)$$

$T_\tau$  is the ordering operator and  $T$  is temperature. The equation of motion for the usual one-electron propagator (5a) contains both functions (5a) and (5b), while the equation of motion for (5b) would contain some two-electron propagators, different from (5b) itself, if one does not make some assumptions. This therefore introduces the possibility to express all two-electron propagators, except (5b), through (5a) and the proper *bonding parameters*

$$G_{im}^\pm(\tau) = G_{im}^\pm(\tau, \tau + 0) = \langle c_{m,\pm\sigma}^\dagger(\tau) c_{i\sigma}(\tau) \rangle \quad (7a)$$

$$\Delta_{im}^\pm(\tau) = \Delta_{im}^\pm(\tau, \tau + 0) = \langle c_{m,\pm\sigma}^\dagger(\tau) c_{i\sigma}(\tau) n_{i,-\sigma}(\tau) \rangle. \quad (7b)$$

(Bonding parameters (7a) with  $i = m$  are occupancy numbers.) Since we are going to study a system with macroscopic oscillations (section 3), we save argument  $\tau$  in (7), indicating a lack of time invariance.

In his pioneer work Hubbard made an assumption, which may be called 'a Hartree-type *ansatz*' (Hubbard 1963). For one of three analogous terms it reads

$$t(\mathbf{r}_{ij})c_{i,-\sigma}^+(\tau)c_{i\sigma}(\tau)c_{m,-\sigma}(\tau) \simeq t(\mathbf{r}_{ij})G_{ii}^-(\tau)c_{m,-\sigma}(\tau). \quad (8a)$$

Hubbard pointed out that 'whatever approximations are made in ... [the terms of type (8a)], one will obtain a theory that goes over into exact solution in the zero bandwidth limit'. (This limit  $|t(\mathbf{r}_{ij})| \ll U$  we call strong correlation.) Instead of (8a) we propose a 'Hartree-Fock-type *ansatz*'

$$t(\mathbf{r}_{ij})c_{i,-\sigma}^+(\tau)c_{i\sigma}(\tau)c_{m,-\sigma}(\tau) \simeq t(\mathbf{r}_{ij})[G_{ii}^-(\tau)c_{m,-\sigma}(\tau) - G_{mi}^+(\tau)c_{i\sigma}(\tau)]. \quad (8b)$$

We think that (8b) generalizes (8a), making use of those bonding parameters which involve two different atomic sites; and that (8b) in the strong correlation limit plays the same role as Hubbard's resonance broadening and scattering corrections, made in order to improve results based on (8a) and analogous approximations (Hubbard 1964). As we remarked earlier, we keep values of the bonding parameters (7) outside the framework of the present theory. They should be calculated or guessed by some other means; however, this must be done self-consistently with the chemical potential  $\mu$  (see section 3).

After linearization (8b) and wavevector transformation, the equations of motion for Green functions (5) become:

$$\begin{aligned} \left(\frac{\partial}{\partial \tau} + \varepsilon_0 + t_k - \mu\right) G_{k,k+q}^\pm(\tau, \tau') + U \Delta_{k,k+q}^\pm(\tau, \tau') &= -\delta(\tau - \tau')\delta^+(q) \\ \left(\frac{\partial}{\partial \tau} + \varepsilon_0 + U - \mu\right) \Delta_{k,k+q}^\pm(\tau, \tau') + \frac{1}{N} \sum_{k_1, q_1} (t_{k+q_1} - t_{k_1+q_1} + t_{k_1}) & \\ \times [G_{k+q_1, k+q}^\pm(\tau, \tau') G_{k_1, k_1+q_1}^\pm(\tau) - G_{k+q_1, k+q}^\mp(\tau, \tau') G_{k_1, k_1+q_1}^\mp(\tau)] & \\ = \mp \delta(\tau - \tau') \frac{1}{N} \sum_{k_1} G_{k_1, k_1+q}^\pm(\tau). & \end{aligned} \quad (9)$$

It is clear that equations (9) simply reflect the structure of decoupling (8b), and thus the formalism itself does not depend on the particular scheme chosen, (8a) or (8b) or some other, though the final solution depends of course on the decoupling. Since the goal of this paper is not to compare different decoupling schemes and their consequences, but rather to demonstrate the work of the equations of motion formalism with respect to collective oscillations dispersion relation, the choice of decoupling is not significant. We simply choose the more general one—(8b).

Equations (9) seem to be useful in the investigation of different collective modes, excited states and susceptibilities to external fields (the last opportunity can be realized after adding the proper interaction function to the diagonal coefficients before  $G_{k,k+q}^\pm(\tau, \tau')$  and  $\Delta_{k,k+q}^\pm(\tau, \tau')$  on the left-hand side of (9)). Working with (9) does not need any elaborate method, because in its structure (9) is analogous to the well studied equations in the theory of superconductivity. The self-oscillatory condition is obtained from (9) in the next section by the same technique as for superconductor susceptibility to a variable external field (Abrikosov *et al* 1963).

### 3. Self-oscillatory condition

We shall develop a theory of  $\omega_{\text{cor}}(\mathbf{q})$  by the following reasoning. Suppose that an infinitesimal external force of frequency  $\omega$  is applied to the system, and this is accounted for in (9) after analytical continuation of time-dependent propagators onto temperature propagators by  $\omega \rightarrow i\omega$ . Then the solution of (9) can be constructed as a superposition of stationary functions ( $G^0, \Delta^0$ ) and small oscillatory functions. It is important that the stationary functions depend on the difference  $(\tau - \tau')$ ; therefore

$$G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{\pm}(\tau, \tau') = G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{0\pm}(\tau - \tau') + G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{1\pm}(\tau - \tau') \exp[-\frac{1}{2}i\omega(\tau + \tau')] \quad (10a)$$

$$G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{\pm}(\tau) = G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{\pm}(\tau, \tau + 0) = G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{0\pm}(-0) + G_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{1\pm}(-0)e^{-i\omega\tau}. \quad (10b)$$

The formulae for Green functions  $\Delta$  (5b) and for bonding parameters (7b) are similar. Inserting (10) into (9) and making use of the smallness of oscillatory parts in (10), one obtains linear equations for  $G^1$  and  $\Delta^1$ . Suppose that from these equations a value  $i\omega = \omega_{\text{cor}}$  and a value of  $\mathbf{q}$  can be extracted, for which values solutions  $G^1$  and  $\Delta^1$  become indefinite and, consequently, independent of the external force. It would mean that the electron system has a collective oscillatory mode, which exists, after it has been excited, without support of the external field. So, we conclude that frequency  $\omega_{\text{cor}}$  and wavevector  $\mathbf{q}$ , found in such a way, belong to the self-oscillatory collective mode. We name a relation, which yields  $\omega_{\text{cor}}(\mathbf{q})$ , a *self-oscillatory condition*. (The damping constant of the oscillatory mode also may be estimated, if one takes account of those non-linear terms, which were considered as small, when subdividing (9) into stationary and oscillatory equations.)

Equations (9) require application of Fourier-transform formalism. Since both propagators (5) have the fermion commutation type, their  $\omega$ - $\tau$  Fourier transform must contain the fermionic frequencies (odd)

$$\omega_n = (2n + 1)\pi T \quad n = 0, \pm 1, \pm 2, \dots \quad (11a)$$

$$f(\tau - \tau') = T \sum_{\omega_n} \exp[-i\omega_n(\tau - \tau')] f(\omega_n) \quad f = G^0, \Delta^0, G, \Delta. \quad (11b)$$

As to the oscillatory functions in (10a), their Fourier frequencies  $\omega'_n$  must obey fermion condition (11a) in combination with  $\omega$ :

$$f^1(\tau - \tau') = T \sum_{\omega'_n} \exp[-i\omega'_n(\tau - \tau')] f^1(\omega'_n) \quad f^1 = G^1, \Delta^1 \quad (12a)$$

$$-i\omega_n(\tau - \tau') = -i\omega'_n(\tau - \tau') - \frac{1}{2}i\omega(\tau + \tau'). \quad (12b)$$

Since  $\tau$  and  $\tau'$  in (12b) are independent variables,  $\tau$  must be a bosonic frequency ( $\omega = 2n_0\pi T$  in accordance with the macroscopic character of the external force used in previous reasoning about the self-oscillatory mode). From (11b) and (12b) it must be concluded that frequencies of oscillatory functions  $G^1$  and  $\Delta^1$  are neither fermionic nor bosonic, but have a mixed character:

$$\omega'_n = (2n + 1 + n_0)\pi T \quad n = 0, \pm 1, \pm 2, \dots, \omega = 2n_0\pi T. \quad (13)$$

With the help of (11) and (12) one can take the motion equations (9) apart, subdividing them into stationary and oscillatory parts. Neglecting all terms containing  $G^1$  and  $\Delta^1$ , we get a stationary part:

$$\begin{aligned}
 &(-i\omega_n + \varepsilon_0 + t_k - \mu)G_{k,k+q}^{0\pm}(\omega_n) + U\Delta_{k,k+q}^{0\pm}(\omega_n) = -\delta^+\delta(q) \\
 &(-i\omega_n + \varepsilon_0 + U - \mu)\Delta_{k,k+q}^{0\pm}(\omega_n) + \frac{1}{N} \sum_{k_1, q_1} (t_{k+q_1} - t_{k_1+q_1} + t_{k_1}) \\
 &\quad \times [G_{k+q_1, k+q}^{0\pm}(\omega_n)G_{k_1, k_1+q_1}^{0+}(-0) - G_{k+q_1, k+q}^{0\mp}(\omega_n)G_{k_1, k_1+q_1}^{0-}(-0)] \\
 &= \mp \frac{1}{N} \sum_{k_1} G_{k_1, k_1+q}^{0\pm}(-0).
 \end{aligned} \tag{14}$$

Neglecting all terms of the second order with respect to  $G^1$ , we get an oscillatory part:

$$\begin{aligned}
 &(-i\omega'_n - \frac{1}{2}i\omega + \varepsilon_0 + t_k - \mu)G_{k,k+q}^{1\pm}(\omega'_n) + U\Delta_{k,k+q}^{1\pm}(\omega'_n) = 0 \\
 &(-i\omega'_n - \frac{1}{2}i\omega + \varepsilon_0 + U - \mu)\Delta_{k,k+q}^{1\pm}(\omega'_n) + \frac{1}{N} \sum_{k_1, q_1} (t_{k+q_1} - t_{k_1+q_1} + t_{k_1}) \\
 &\quad \times [G_{k+q_1, k+q}^{1\pm}(\omega'_n)G_{k_1, k_1+q_1}^{0+}(-0) - G_{k+q_1, k+q}^{1\mp}(\omega'_n)G_{k_1, k_1+q_1}^{0-}(-0)] \\
 &= \frac{1}{N} \sum_{k_1} \mp G_{k_1, k_1+q}^{1\pm}(-0) - \sum_{q_1} (t_{k+q_1} - t_{k_1+q_1} + t_{k_1}) \\
 &\quad \times [G_{k+q_1, k+q}^{0\pm}(\omega'_n - \omega/2)G_{k_1, k_1+q_1}^{1+}(-0) - G_{k+q_1, k+q}^{0\mp}(\omega'_n - \omega/2)G_{k_1, k_1+q_1}^{1-}(-0)].
 \end{aligned} \tag{15}$$

Self-oscillatory equations (15) are basic for  $\omega_{\text{cor}}(q)$  calculation. According to the previous reasoning, we have to find a condition for  $\omega$  and  $q$  such that equations (15) give an indefinite solution. Suppose stationary propagators are known. Then we can express stationary and oscillatory functions of  $\tau$  (10b) by the reciprocal Fourier transform as

$$G_{k,k+q}^{1\pm}(-0) = T \sum_{\omega'_n} G_{k,k+q}^{1\pm}(\omega'_n) \quad G_{k,k+q}^{0\pm}(-0) = T \sum_{\omega_n} G_{k,k+q}^{0\pm}(\omega_n) \tag{16}$$

and can subdivide (7) into stationary and oscillatory bonding parameters

$$f_q^\pm = \frac{1}{N} \sum_k f_{k,k+q}^\pm(-0) \quad f = G^0, \Delta^0, G^1, \Delta^1. \tag{17}$$

We conclude that if we reduce equations (15) to a linear system with unknown oscillatory bonding parameters  $G^{1+}$ ,  $G^{1-}$ ,  $\Delta^{1+}$  and  $\Delta^{1-}$ , defined by (17), then we obtain the self-oscillatory condition as an equality of the system's main determinant to zero.

In order to derive the self-oscillatory condition from (15), we have to know stationary propagators  $G_{k,k+q}^{0\pm}(\omega_n)$  and  $\Delta_{k,k+q}^{0\pm}(\omega_n)$ , which may be obtained self-consistently from (14) and (16). The loop of the self-consistency starts with the initial *a priori* guess for  $G_{k,k+q}^{0\pm}(-0)$ . Then linear system (14) is solved, giving energy spectrum  $\varepsilon_i(k, k+q)$  and propagator  $G_{k,k+q}^{0\pm}(\omega_n)$ , both quantities depending on  $\mu$  and  $T$ . After that, summation (16) is performed, and from here the loop of self-consistency begins again.

Thus, we have in principle two possibilities:

(i) We can find a value of  $\mu$  consistent with *a priori* chosen bonding parameters.

(ii) On the other hand, we can make bonding parameters consistent with the value of  $\mu$  chosen in advance.

We make a note about this item. Of course, equations (14), written on the basis of (8b), do not describe exactly all the possible phases of strongly correlated systems. However, (14) is valid for any set of bonding parameters  $G_{k,k+q}^{0\pm}(-0)$ , which defines sufficiently a systems' ordering and other thermal equilibrium properties. Applying approach (i) to the exact set of  $G_{k,k+q}^{0\pm}(-0)$ , we get from (14) a value of  $\mu$  that may be in poor agreement with the exact theory. We can take the discrepancy of  $\mu$  as a measure of error of (14)–(15). Another situation can be imagined, when the precision of the  $\mu$  value is more important than precision of some  $G_{k,k+q}^{0\pm}(-0)$  values. For example,  $\mu$  may define a metallic or insulating occupancy. In such a case we apply approach (ii) and find from (14) a self-consistent set of bonding parameters for given  $\mu$  and occupancy. The discrepancy of the density of states or some other quantity, connected with  $G_{k,k+q}^{0\pm}(-0)$ , may estimate the error of (14)–(15).

#### 4. Self-oscillatory condition for a system with a translationally invariant ground state

Simple systems must be studied first, so we shall apply (14) and (15) to the case of a system with a translationally invariant ground state, i.e. we assume that stationary bonding parameters depend only on inter-site distance

$$G_{ij}^{0\pm}(-0) = G_{r_{ij}}^{0\pm} \quad \Rightarrow \quad G_{k,k+q}^{0\pm}(-0) = G_k^{0\pm} \delta(q) \quad G_k^{0\pm} = \frac{1}{N} \sum_k G_k^{0\pm}. \quad (18)$$

So in this case we define a stationary state with a pair of site-independent occupancy numbers  $G^{0\pm} = \langle c_{i\sigma}^+ c_{i\pm\sigma} \rangle$  and chemical potential  $\mu$  (at temperature  $T$ ).

It may be noted that another interesting case would be a system with a charge- or spin-wave ordering:

$$G_{ij}^{0\pm}(-0) = G_{r_{ij}}^{0\pm} \exp(ir_{ij}Q) \quad \Rightarrow \quad G_{k,k+q}^{0\pm}(-0) = G_{k-Q}^{0\pm} \delta(q - Q). \quad (19)$$

For the remaining part of this paper we consider case (18) only, and presume that the system obeys (14) in thermodynamic equilibrium.

Substituting (18) into (14) yields the stationary propagator

$$G_k^{0\pm}(\omega_n) = |D_k^\pm(\omega_n)| / |D_k(\omega_n)| \quad (20)$$

where  $4 \times 4$  matrices in determinants of denominator and numerator can be obtained by

$$D_k(E) = \begin{vmatrix} X_k(E) & 0 & U & 0 \\ 0 & X_k(E) & 0 & U \\ t_k G^{0+} & -t_k G^{0-} & Y(E) & 0 \\ -t_k G^{0-} & t_k G^{0+} & 0 & Y(E) \end{vmatrix} \quad d = \begin{vmatrix} -1 \\ 0 \\ -G^{0+} \\ G^{0-} \end{vmatrix} \quad (21)$$

$$\begin{matrix} \uparrow & \uparrow \\ D_k^+(E) & D_k^-(E) \end{matrix} \quad \leftrightarrow$$

$$X_k(E) = -E + \varepsilon_0 + t_k - \mu \quad Y(E) = -E + \varepsilon_0 + U - \mu.$$

(After changing its first or second column by  $d$ , as arrows in (21) show,  $D_k(E)$  transforms into  $D_k^+(E)$  or  $D_k^-(E)$ .) Energy poles of (20) are

$$|D_k(E)| = \prod_{m=1}^4 [E - \varepsilon_m(k) + \mu] \quad (22a)$$

$$\varepsilon_m(k) = \varepsilon_0 + (U + t_k)/2 \pm [(U - t_k)^2/4 + Ut_k(G^{0+} \pm G^{0-})]^{1/2}. \quad (22b)$$

Self-consistency of  $G^{0\pm}$  and  $\mu$  is established by substituting (20) into (17):

$$G^{0\pm} = \frac{1}{N} \sum_k G_k^{0\pm} \quad (23a)$$

$$G_k^{0\pm} = T \sum_{\omega_n} |D_k^{\pm}(\omega_n)| / |D_k(\omega_n)|. \quad (23b)$$

Frequency summation in (23b) is performed by the well known formula of the temperature Green function theory (Abrikosov *et al* 1963)

$$T \sum_{\omega_n} f(i\omega_n) \frac{1}{i\omega_n - \varepsilon + \mu} = \frac{1}{2} f(\varepsilon - \mu) \tanh \left( \frac{\mu - \varepsilon}{2T} \right). \quad (24)$$

Applying (24) to (23b), one must remember that energy spectrum (22b) may be doubly degenerate in some  $k$ -points, because of the second  $\pm$  sign in (22b). For the case of non-degenerate set  $\{\varepsilon_l(k)\}$  frequency summation in (23b) is easily performed by (24), giving

$$G_k^{0\pm} = \frac{1}{2} \sum_m \frac{|D_k^{\pm}(\varepsilon_m(k) - \mu)|}{\prod_{l \neq m} [\varepsilon_m(k) - \varepsilon_l(k)]} \tanh \left( \frac{\mu - \varepsilon_m(k)}{2T} \right). \quad (25)$$

If degeneracy occurs, then indefiniteness 0/0 arises in (25). We treat this case in the appendix.

Using matrix expressions (20) and (21) we reduce (15) to the self-oscillatory condition after changing its unknowns from propagators  $G_{k,k+q}^{1\pm}(\omega'_n)$  to bonding parameters  $G_q^{1\pm}$ . First we exclude  $\Delta_{k,k+q}^{1\pm}(\omega'_n)$ , substituting the first equation (15) into the second. Applying translationally invariant case conditions (18) we obtain

$$\begin{aligned} & \frac{1}{U} \left\| \begin{array}{cc} Ut_k G^{0+} - X_k(i\omega'_n + i\omega/2) Y(i\omega'_n + i\omega/2) & -Ut_k G^{0-} \\ -Ut_k G^{0-} & Ut_k G^{0+} - X_k(i\omega'_n + i\omega/2) Y(i\omega'_n + i\omega/2) \end{array} \right\| \\ & \times \left\| \begin{array}{c} G_{k,k+q}^{1+}(\omega'_n) \\ G_{k,k+q}^{1-}(\omega'_n) \end{array} \right\| \\ & = \left\| \begin{array}{cc} -1 - t_k G_{k+q}^{0+}(\omega'_n - \omega/2) & t_k G_{k+q}^{0-}(\omega'_n - \omega/2) \\ -t_k G_{k+q}^{0-}(\omega'_n - \omega/2) & 1 + t_k G_{k+q}^{0+}(\omega'_n - \omega/2) \end{array} \right\| \left\| \begin{array}{c} G_q^{1+} \\ G_q^{1-} \end{array} \right\| \end{aligned} \quad (26)$$

where we write the same auxiliary functions  $X_k(E)$  and  $Y(E)$  as in (21). We note that the  $2 \times 2$  matrix on the left-hand side of (26) has a determinant equal to  $|D_k(i\omega'_n + i\omega/2)|$ —this will appear in (28b) through the inverse matrix as

$$\left\| \begin{array}{cc} a & b \\ b & a \end{array} \right\|^{-1} = \left| \begin{array}{cc} a & b \\ b & a \end{array} \right|^{-1} \left\| \begin{array}{cc} a & -b \\ -b & a \end{array} \right\|. \quad (27)$$



It is clear that frequency and wavevector summations (16) and (17) can be performed in (26), if we express the vector of propagators on the left-hand side of (26) through the vector of bonding parameters on the right-hand side. We do it with the help of (27) and (20). The result is

$$\left\| \begin{array}{c} G_{k,k+q}^{1+}(\omega'_n) \\ G_{k,k+q}^{1-}(\omega'_n) \end{array} \right\| = R_{kq}(i\omega'_n, i\omega) \left\| \begin{array}{c} G_q^{1+} \\ G_q^{1-} \end{array} \right\| \quad (28a)$$

$$R_{kq}(i\omega'_n, i\omega) = \frac{A_k(i\omega'_n + i\omega/2)B_{kq}(i\omega'_n - i\omega/2)}{|D_k(i\omega'_n + i\omega/2)||D_{k+q}(i\omega'_n - i\omega/2)|}. \quad (28b)$$

The  $2 \times 2$  matrix  $A_k(i\omega'_n + i\omega/2)$  is derived in the course of matrix inversion (27) of the left-hand side of (26):

$$A_k(E) = \left\| \begin{array}{cc} Ut_k G^{0+} - X_k(E)Y(E) & -Ut_k G^{0-} \\ -Ut_k G^{0-} & Ut_k G^{0+} - X_k(E)Y(E) \end{array} \right\|. \quad (29)$$

The  $2 \times 2$  matrix  $B_{kq}(i\omega'_n - i\omega/2)$  is obtained after incorporating (20) into the matrix of the right-hand side of (26):

$$B_{kq}(E) = \left\| \begin{array}{cc} -|D_{k+q}(E)| - t_k |D_{k+q}^+(E)| & t_k |D_{k+q}^-(E)| \\ -t_k |D_{k+q}^-(E)| & |D_{k+q}(E)| + t_k |D_{k+q}^+(E)| \end{array} \right\|. \quad (30)$$

The self-oscillatory condition comes out strictly from (28) as a condition for the non-trivial indefinite solution of the linear system with unknown oscillatory bonding parameters (17) as the equality of the main  $2 \times 2$  determinant to zero:

$$\left| \frac{1}{N} \sum_k R_{kq}(i\omega) - \mathbf{I} \right| = 0 \quad (31a)$$

$$R_{kq}(i\omega) = T \sum_{\omega'_n} R_{kq}(i\omega'_n, i\omega) \quad (31b)$$

where  $\mathbf{I}$  is the  $2 \times 2$  unit matrix.

The task of frequency summation in (31b) resembles the previous one (23)–(25). The energy poles in (31b) are  $i\omega'_n = \varepsilon_m(k) - i\omega/2$  and  $i\omega'_n = \varepsilon_m(k+q) + i\omega/2$  (see (28b) and (22a)). Thus we have to express the frequency sum (31b) through terms of the type (24):

$$T \sum_{\omega'_n} \frac{a(i\omega'_n + i\omega/2)b(i\omega'_n - i\omega/2)}{i\omega'_n \pm i\omega/2 - \varepsilon + \mu} = \frac{1}{2} \tanh\left(\frac{\mu - \varepsilon}{2T}\right) \times \begin{cases} a(\varepsilon - \mu)b(\varepsilon - i\omega - \mu) \\ a(\varepsilon + i\omega - \mu)b(\varepsilon - \mu). \end{cases} \quad (32)$$

Applying (32) to the summation in (31b) after substitution (28b), we get the final formula, which we write here for the case of non-degenerate one-electron spectrum (22) in  $k$  and in  $(k+q)$  points:

$$R_{kq}(\omega) = \frac{U}{2} \sum_m \sum_{m'} \frac{1}{(\omega - \varepsilon_m + \varepsilon'_{m'}) \prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell) \prod_{\ell' \neq m'} (\varepsilon'_{m'} - \varepsilon'_{\ell'})} \\ \times \left[ -\tanh\left(\frac{\mu - \varepsilon_m}{2T}\right) A_k(\varepsilon_m - \mu) B_{kq}(\varepsilon_m - \omega - \mu) \right. \\ \left. + \tanh\left(\frac{\mu - \varepsilon'_{m'}}{2T}\right) A_k(\varepsilon'_{m'} + \omega - \mu) B_{kq}(\varepsilon'_{m'} - \mu) \right] \quad (33)$$

with

$$\varepsilon_m = \varepsilon_m(\mathbf{k}) \quad \varepsilon'_{m'} = \varepsilon_{m'}(\mathbf{k} + \mathbf{q}).$$

Analytical continuation  $\omega \rightarrow i\omega$  in (31b) becomes a trivial change of argument after applying (32). We have done this change in (33). Degenerate cases are considered in the appendix.

The self-oscillatory condition (31a) has the form of a determinant equation on wavevector  $\mathbf{q}$  and frequency  $\omega_{\text{cor}} \rightarrow i\omega$ . This condition describes a system with translationally invariant ground state, characterized by a pair of occupancy numbers  $G^{0\pm}$ . The kernel matrix (33) of the self-oscillatory condition shows a close resemblance to the analogous plasmon expression (Doniach and Sondheimer 1974). Consider the left-hand side of (31a) as a function of frequency. It is seen that there is a quasi-continuum of poles, which describes one-electron excitations:  $\omega_{\mathbf{k}\mathbf{q}} = \varepsilon_m(\mathbf{k}) - \varepsilon_{m'}(\mathbf{k} + \mathbf{q})$ . But when  $\omega$  exceeds the upper limit of  $\omega_{\mathbf{k}\mathbf{q}}$ , the left-hand side function of  $\omega$  in (31a) becomes analytical, and (31a) can be solved rather easily, because it does not need any self-consistent procedure. A solution  $\omega_{\text{cor}}$  of (31a) at a given  $\mathbf{q}$  (if it exists), which is split off from the continuum  $\omega_{\mathbf{k}\mathbf{q}}$ , is a frequency of the collective mode, as was formulated in section 3.

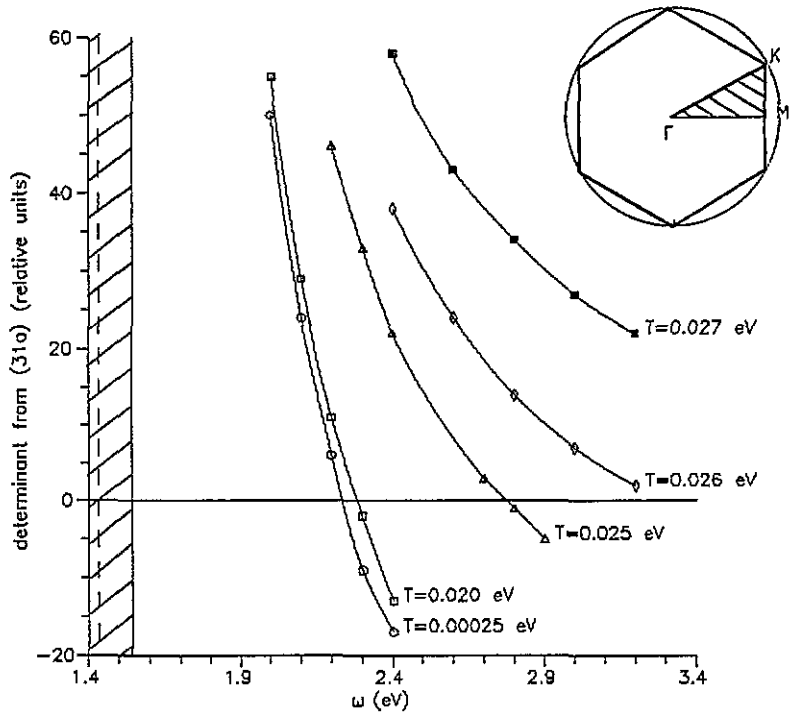
Equation (31a) is more convenient for a numerical solution than for an analytical one. The calculations were performed by the author and will be described in section 5 in connection with possible experimental evidence. In order to illustrate the behaviour of  $\omega_{\text{cor}}(\mathbf{q})$  as it follows from analysis of the denominator of (33), we attract the reader's attention to figure 1 with the graph of determinant from (31a) as a function of  $i\omega$  (the intersection with the horizontal line gives a graphic solution for  $\omega_{\text{cor}}$ ).

## 5. Possible experimental evidence

In this section we try to explain some spectroscopic data on the surfaces Si(111)1  $\times$  1 and 7  $\times$  7 on the basis of the assumption that correlation oscillations occur in this two-dimensional electron system of dangling bonds. The strongly correlated character of pure Si(111) in its 1  $\times$  1 and 7  $\times$  7 reconstructions is well established. For example, it was shown theoretically that the 1  $\times$  1 phase is unstable with respect to charge- and spin-wave ordering transition, while a strong one-site correlation of dangling-bond electrons is the main cause of this behaviour (Muramatsu and Hanke 1984). The experiments proved that the electron structure of both 1  $\times$  1 and 7  $\times$  7 reconstructions may be described by the Hubbard model with insulator occupancy over a wide temperature range (Yokotsuka *et al* 1983).

We want to discuss some results of ARUPS (angle-resolved ultraviolet photoemission spectroscopy), HREELS (high-resolution electron-energy-loss spectroscopy), inverse photoemission (bremsstrahlung spectroscopy) and optical response spectroscopy.

An energy-loss peak was found on Si(111)7  $\times$  7 with wide dispersion (from 1 to 1.8 eV) in the Brillouin zone, and was assigned to electron transitions between a pair of surface-state bands (Layet *et al* 1984). The average energy-loss value agrees with one of the surface-state band transition energies, which have been measured by ARUPS for occupied bands (Uhrberg *et al* 1985) and by inverse photoemission for the empty band (Himpfel and Fauster 1984). Meanwhile, ARUPS had not shown any dispersion of the occupied surface-state band comparable with 0.8 eV dispersion of the HREELS peak. Therefore, the mechanism of the surface-band transition does not seem to be a very good explanation of HREELS data considered. On the other hand, energy-loss spectra usually contain collective excitation modes (such as plasmons), while ARUPS naturally does not. Thus, it seems



**Figure 1.** Graphic numerical solution of dispersion relation (31a) for a two-dimensional perfect triangular lattice with translationally invariant, paramagnetic ground state at different temperatures  $T$ . Wavevector  $q$  of a solution was fixed at the K-point of the Brillouin zone (shown near the graph, the irreducible part is shaded). The parameters of the model gave a paramagnetic, insulating ground state:  $G^{0\pm} = 1/2$ ,  $\varepsilon_0 = -1$  eV,  $\mu = 0$ ,  $t(\tau_{ij}) = t = 0.0125$  eV for the nearest-neighbour sites  $i, j$ . Chemical potential was situated in the Hubbard energy gap:  $|\mu - \varepsilon_i(k)| \geq 0.39$  eV. The shaded area in the graph shows the continuum of one-electron excitations  $\omega_{kq} \leq 1.54$  eV. Correlation parameter  $U$  may be considered as the energy scale of the model; its value is shown by the vertical dashed line.

reasonable to test the correlation oscillations mechanism for the broad-dispersion HREELS peak of Si(111)7  $\times$  7.

We have performed non-self-consistent calculations of  $\omega_{\text{cor}}(q)$  in order to prove two items:

(i) that  $\omega_{\text{cor}}(q)$  may have the same order of value as HREELS shows for Si(111)7  $\times$  7; and

(ii) that the dispersion of  $\omega_{\text{cor}}(q)$  may be wide, while the one-electron band  $t_k$  (3)–(4) is narrow.

The details of the calculations were published previously (Moliver 1991). The model was considered with a translationally invariant, paramagnetic ground state:  $G^{0\pm} = 1/2$ . The correlation parameter was chosen according to the model of Si(111) (Louis *et al* 1982, 1983):  $U = 1.43$  eV. The nearest-neighbour approximation was applied with different values of  $t = 0.0125$  to 0.1 eV. The chemical potential  $\mu$  was placed non-self-consistently in the middle of the energy gap between Hubbard bands (22b). Then  $\omega_{\text{cor}}(q)$  was calculated along high-symmetry directions of the Brillouin zone of the perfect triangular two-dimensional lattice, and both propositions (i) and (ii) were proved (figure 2).

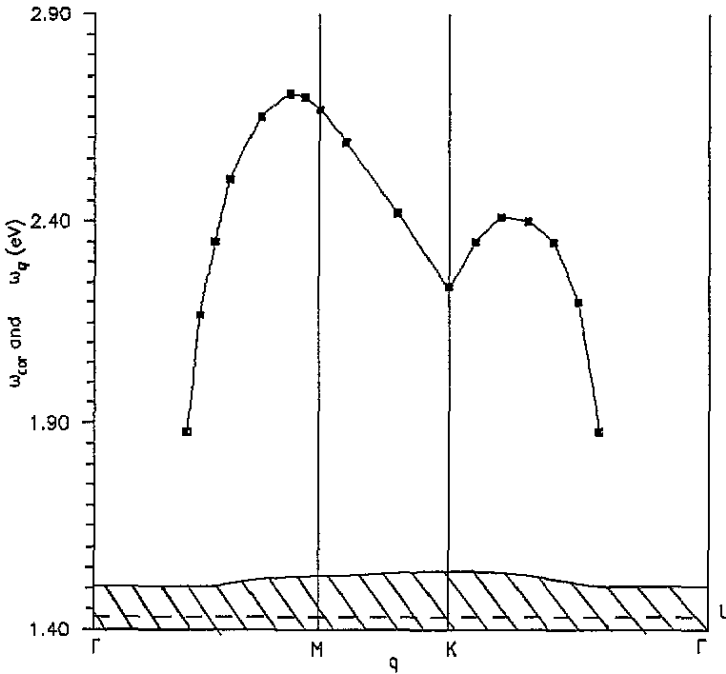


Figure 2. Band diagram of correlation oscillation mode along the boundaries of the irreducible part of the Brillouin zone. The shaded area shows frequencies and momentum transfers of Hubbard interband transitions according to

$$\omega_q \leq \max_{k,i,j} \{\varepsilon_i(k) - \varepsilon_j(k+q)\}.$$

Temperature  $T = 0.00025 \text{ eV} \simeq 3 \text{ K}$ ; other parameters are the same as in figure 1. Horizontal dashed line shows the energy scale of the model  $U$ .

The calculations also showed that the temperature behaviour of the correlation oscillation frequency has the character of a phase transition: at  $T \rightarrow (T_c - 0)$ ,  $\omega_{\text{cor}}(q) \rightarrow \infty$ , while at  $T > T_c$  oscillations do not exist. The critical temperature  $T_c$  depends on the bandwidth and varies from  $T_c \simeq 2t$  for  $t \simeq 0.0125 \text{ eV}$  to  $T_c \simeq 0.041 \text{ eV}$  for  $t > 0.075 \text{ eV}$  (figure 3). The occurrence of the critical behaviour, the range of  $T_c$ , the dependence of  $T_c$  on a single parameter of the Hubbard model  $U/t$ , all these properties of  $\omega_{\text{cor}}(q)$  may be considered as reflecting the situation with the reconstruction transitions  $1 \times 1 \leftrightarrow 7 \times 7$  on Si(111) and the interpretation of these transitions with a single-parameter Hubbard model (Yokotsuka *et al* 1983).

In HREELS experiment on Si(111)  $7 \times 7$  the width of the elastic scattering peak tail (near-elastic energy losses) was explained by multiple dipole scattering from surface plasmons, created by electrons of an extremely narrow surface-state band (width of the band 1 meV, effective mass  $60m$ ) (Persson and Demuth 1984). It seems impossible to exclude many-electron effects from such a narrow-band model, so the idea of scattering from correlation oscillation excitations was tested (Moliver 1991). We estimate the probability of the single scattering process with energy loss  $E$  and momentum transfer  $p$  from the previously excited correlation oscillation as

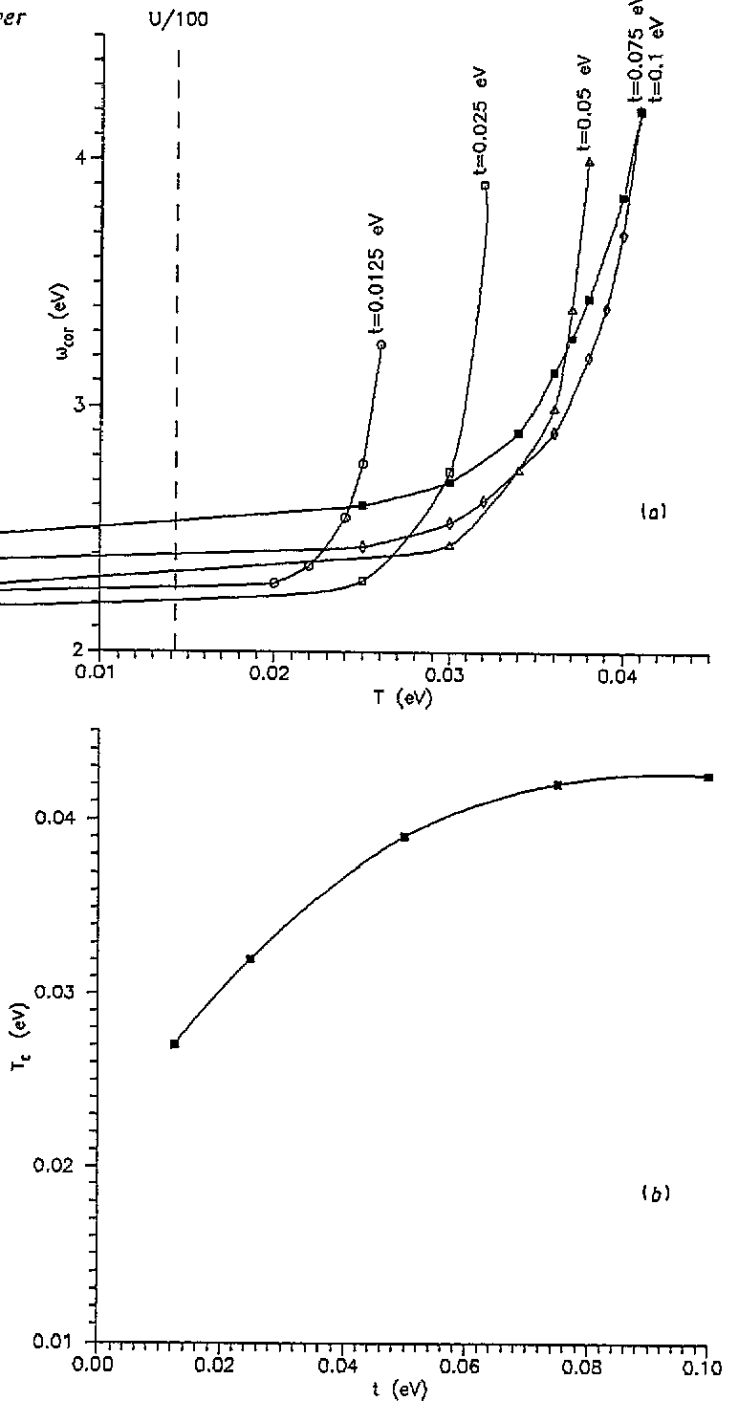


Figure 3. (a) Temperature dependence of correlation oscillation frequency at different values of the hopping integral  $t$ . Critical temperature  $T_c$ , at which  $\omega_{\text{cor}}(q) \rightarrow \infty$ , can be estimated graphically. (Vertical dashed line shows energy scale of the model  $U/100$ .) (b) Phase diagram of correlation oscillation regime for a strongly correlated system with translationally invariant, paramagnetic ground state. In the area under the phase line the correlation oscillations may be excited; in the area above, oscillations do not exist (equation (31a) has no solution). The parameters of the model (except  $t$ ) were the same as in figures 1 and 2. The wavevector  $q$  was fixed in the K-point of the Brillouin zone. The whole phase plane corresponds to the insulating ground state:  $2T \leq 0.1 \text{ eV} \ll 0.39 \text{ eV} \leq |\mu - \varepsilon_i(k)|$ .

$$P(E, \mathbf{p}) \propto \int d^2\mathbf{q} \delta[E - \omega_{\text{cor}}(\mathbf{q}) + \omega_{\text{cor}}(\mathbf{q} + \mathbf{p})] \quad (34)$$

and found, considering the calculated spectrum of  $\omega_{\text{cor}}(\mathbf{q})$ , that (34) has a logarithmically wide tail at near-elastic conditions of HREELS experiment  $E \rightarrow 0$ ,  $\mathbf{p} \rightarrow 0$ :

$$P(E, \mathbf{p}) \propto \frac{1}{|\mathbf{p}|} \ln \left( \frac{c|\mathbf{p}| + (c\mathbf{p}^2 - E^2)^{1/2}}{E} \right) \quad c = \max |\nabla_{\mathbf{q}} \omega_{\text{cor}}(\mathbf{q})|. \quad (35)$$

Since the incident electron beam in HREELS has enough energy to excite the correlation oscillations, the scattering process (34) can occur, and quasi-elastic energy losses may be analysed using dipole scattering theory (Persson and Demuth 1984) together with (35), which does not need unrealistic surface-state band parameters.

Recently several singularities were found in the Si(111)7 × 7 optical reflectance spectrum, which were explained by electron surface-state inter-band transitions (Alameh and Borensztein 1991). One of these optical response singularities (at  $h\nu = 1.8$  eV) coincides very well with the HREELS energy-loss peak, discussed above (Layet *et al* 1984, Persson and Demuth 1984), but the other one (at  $h\nu = 2.5$  eV) is completely absent in HREELS. This corresponds with the correlation oscillation explanation of HREELS peak proposed above, because the efficiencies of collective mode excitation and of one-electron transition stimulation by incident electron must be different. In fact, EELS is well known for its high sensitivity to bulk and surface plasmon collective modes.

## 6. Conclusion

A strongly correlated electron system has a collective oscillation mode of bosonic type. Like a plasmon one, this mode shows itself through oscillations of occupancy numbers and other bonding parameters (7a) and (10b). Unlike for the plasmon mode, the electron density of a collective correlation mode cannot be considered apart from the two-electron (correlation) thermodynamic averages (7b). The dispersion relation between frequency and wavevector of the collective correlation mode has been found from the self-oscillatory condition, applied to the Green functions equations of motion.

The closed form of the equations of motion and the consequent self-oscillatory condition have been developed for strongly correlated system (the tight-binding bands of which are much more narrow than the one-site correlation energy). In order to produce the self-oscillatory condition, different cut-off methods may be applied to the series of equations of motion (section 2); several-band models may also be treated in a similar way as the single-band model has been (section 3).

For the strongly correlated system (18) with translationally invariant ground state, the self-oscillatory condition (31a) has a form similar to the plasmon one, but the structure of the kernel is different. The strong connection between occupancy numbers (7a) and their correlation partners (7b) makes the kernel a determinant, the size of which equals the number of independent bonding parameters. For the simple system (18) two occupancy numbers  $G^{0\pm}$  are enough, and thus the self-oscillatory condition has been expressed through the 2 × 2 matrixes (29), (30) and (21).

In search of experimental evidence of the correlation oscillations, some Si(111) dangling-bond surface spectra were studied. The wide-dispersion energy-loss peak (1–1.8 eV through the Brillouin zone) from Si(111)7 × 7 has been explained by excitation of correlation oscillations in a narrow-band strongly correlated system. This explanation agrees

quantitatively with the HREELS data and eliminates the contradiction between the HREELS and the ARUPS interpretations.

The theory presented may be of use in the experimental study of strongly correlated systems. For example, values of the bonding parameters and their wavevector dependence may be 'tested' by calculation and observation of  $\omega_{\text{cor}}(\mathbf{q})$ , giving information about equilibrium state ordering. The critical behaviour of correlation oscillations, found in calculations of  $\omega_{\text{cor}}(\mathbf{q})$  for the single-band system with translationally invariant paramagnetic ground state, 'goes in parallel' with the interpretation of ARUPS data about  $\text{Si}(111)1 \times 1 \leftrightarrow 7 \times 7$  reconstruction transitions on the basis of a single-parameter Hubbard model.

### Acknowledgments

The computations presented in this paper have been carried out at the computer centre of Riga Technical University. I wish to thank A L Shluger and all the colleagues from his seminar at the University of Latvia for fruitful discussions. I am grateful to N N Kristofel (Institute of Physics of Estonia, Tartu) for his interest in this work and helpful comments.

### Appendix. Rules of summation over degenerate one-electron spectrum in (25) and (33)

We reserve indices  $i$  and  $j$  for two degenerate energies (22), index  $m$  for two non-degenerate ones, and index  $\ell$  for all energies:

$$\varepsilon_i(\mathbf{k}) = \varepsilon_j(\mathbf{k}) \neq \varepsilon_m(\mathbf{k}).$$

A pair of terms ( $i$ th and  $j$ th) in sum  $\sum_m$  in (25) must be changed by a single term as follows:

$$\sum_m \frac{f(\varepsilon_m)}{\prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell)} \Rightarrow \sum'_{m \neq i, j} \frac{f(\varepsilon_m)}{\prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell)} + \frac{1}{\prod'_{m \neq i, j} (\varepsilon_i - \varepsilon_m)} \frac{d}{d\varepsilon} f(\varepsilon) \Big|_{\varepsilon = \varepsilon_i = \varepsilon_j}. \quad (\text{A1})$$

If degeneracy occurs in only one of the points  $\mathbf{k}$  or  $(\mathbf{k} + \mathbf{q})$ , then a pair of terms in sum  $\sum_m$  or in  $\sum_{m'}$  of (33) must be treated according to the rule (A1). If both  $\mathbf{k}$  and  $(\mathbf{k} + \mathbf{q})$  points are degenerate, then (A1) must be applied twice:

$$\begin{aligned} & \sum_m \sum_{m'} \frac{f(\varepsilon_m, \varepsilon'_{m'})}{\prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell) \prod_{\ell' \neq m'} (\varepsilon'_{m'} - \varepsilon'_{\ell'})} \\ & \Rightarrow \sum'_{m \neq i, j} \sum'_{m' \neq i', j'} \frac{f(\varepsilon_m, \varepsilon'_{m'})}{\prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell) \prod_{\ell' \neq m'} (\varepsilon'_{m'} - \varepsilon'_{\ell'})} \\ & + \sum'_{m' \neq i', j'} \frac{1}{\prod_{\ell' \neq m'} (\varepsilon'_{m'} - \varepsilon'_{\ell'}) \prod_{m \neq i, j} (\varepsilon_i - \varepsilon_m)} \frac{d}{d\varepsilon} f(\varepsilon, \varepsilon'_{m'}) \Big|_{\varepsilon = \varepsilon_i = \varepsilon_j} \\ & + \sum'_{m \neq i, j} \frac{1}{\prod_{\ell \neq m} (\varepsilon_m - \varepsilon_\ell) \prod'_{m' \neq i', j'} (\varepsilon'_{i'} - \varepsilon'_{m'})} \frac{d}{d\varepsilon} f(\varepsilon_m, \varepsilon') \Big|_{\varepsilon' = \varepsilon'_{i'} = \varepsilon'_{j'}} \\ & + \frac{1}{\prod'_{m \neq i, j} (\varepsilon_i - \varepsilon_m) \prod'_{m' \neq i', j'} (\varepsilon'_{i'} - \varepsilon'_{m'})} \frac{d^2}{d\varepsilon^2} f(\varepsilon, \varepsilon') \Big|_{\substack{\varepsilon = \varepsilon_i = \varepsilon_j \\ \varepsilon' = \varepsilon'_{i'} = \varepsilon'_{j'}}} \quad (\text{A2}) \end{aligned}$$

with

$$\varepsilon_m = \varepsilon_m(\mathbf{k}) \quad \varepsilon_{m'}' = \varepsilon_{m'}(\mathbf{k} + \mathbf{q}).$$

It may be noted that the problem of summation over the degenerate one-electron spectrum, solved by (A1) and (A2), can be by-passed in computational practice. To decide the task of self-consistent definition of  $G^{0\pm}$  and  $\mu$  (23)–(25), or to find  $\omega_{\text{cor}}(\mathbf{q})$  from (31a), one does not need frequency sums (23b) or (31b) themselves. If summation over the Brillouin zone in (23a) and (31a) is performed by the net of  $\mathbf{k}$ -points, then one may simply exclude those points in which formulae (25) and (33) must be treated according to (A1) or (A2). The error of such a simplification can be made small by increasing the density of the  $\mathbf{k}$ -point net (Moliver 1991).

## References

- Abrikosov A A, Gor'kov L P and Dzyaloshinskii I E 1963 *Methods of Quantum Field Theory in Statistical Physics* (Englewood Cliffs, NJ: Prentice-Hall)
- Alameh R and Borensztein Y 1991 *Surf. Sci.* **251/252** 396
- Doniach S and Sondheimer E H 1974 *Green's Functions for Solid State Physicists* (Reading, MA: Benjamin)
- Himpel F J and Fauster Th J 1984 *J. Vac. Sci. Technol. A* **2** 815
- Hubbard J 1963 *Proc. R. Soc. A* **276** 238
- 1964 *Proc. R. Soc. A* **281** 401
- Layet J M, Hoarau J Y, Lüth H and Derrien J 1984 *Phys. Rev. B* **30** 7335
- Louis E, Flores F, Guinea F and Tejedor C 1982 *Solid State Commun.* **44** 1633
- Louis E, Tejedor C and Flores F 1983 *Solid State Commun.* **47** 939
- Moliver S S 1989 *Surface: Physics, Chemistry, Mechanics (Moscow)* No 5, p 64 (in Russian)
- 1991 *Surface: Physics, Chemistry, Mechanics (Moscow)* No 1, p 55 (in Russian)
- Muramatsu A and Hanke W 1984 *Phys. Rep.* **113** 97
- Persson B N J and Demuth J E 1984 *Phys. Rev. B* **30** 5968
- Uhrberg R I G, Hansson G V, Nicholls J M, Persson P E S and Flodström S A 1985 *Phys. Rev. B* **31** 3805
- Yokotsuka T, Kono S, Suzuki S and Sagawa T 1983 *Solid State Commun.* **46** 401