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A MODEL WITH LOCAL ANHARMONICITY IN THEORY OF HTSC SYSTEMS: CORRELATION FUNCTIONS AND "TRANSVERSE" DIELECTRIC SUSCEPTIBILITY

I. V. Stasyuk, A. M. Shvaika

Institute for Condensed Matter Physics
of the Ukrainian National Academy of Sciences
1 Svientsitskii St., UA–290011 Lviv, Ukraine

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Abstract

The calculation of the "transverse" dielectric susceptibility of Hubbard model including interaction with anharmonic vibrations (pseudospins) is performed using the expressions for correlation functions obtained in the generalized random phase approximation. The analysis of possible ferroelectric type anomalies is performed and the temperatures of instabilities T^* are calculated. A phase diagram $T^* - n$ is plotted. The possible interpretation of the onset of superconducting phase in HTSC crystals is proposed.

1 Introduction

In last years in the theory of high–temperature superconducting crystals considerable attention has been payed to the models taking into account, on the one hand, the strong single–site electron correlation in the spirit of Hubbard model and, on the other hand, the interaction with local anharmonic mode of lattice vibrations. Particularly, such properties are typical for vibrations of the so-called apex oxygen ions of the layered compounds of YBaCuO–type structure (see, [1–3]). In the case of local double–well potential, the vibrational degrees of freedom can be presented by pseudospin variables. The Hamiltonian of the pseudospin–electron model derived in this way (so-called Müller model) has the following form [4]

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma}, \tag{1.1}$$

where t_{ij} being terms describing the electron transfer. The single–site part H_i includes the electron correlation (U–term), interaction with anharmonic mode (g–term), the energy of the tunneling splitting (Ω–term) and energy of the anharmonic potential asymmetry (h–term)

$$H_i = U n_{i\uparrow} n_{i\downarrow} + E_0(n_{i\uparrow} + n_{i\downarrow}) + g(n_{i\uparrow} + n_{i\downarrow})S_i^z - \Omega S_i^x - h S_i^z. \tag{1.2}$$

Here, E_0 gives the origin for energies of the electron states at lattice sites.

Hamiltonian of (1.1)-type can be obtained considering excitonic mechanism of superconductivity [5]. It was proposed in [6] as a model for the consideration of electron states and effective electron-electron interactions by means of cluster calculations. The investigations of possible superconducting pair correlations were performed in the framework of model (1.1) using numerical Monte-Carlo simulation [7].

In previous papers [8,9], we considered single-electron spectrum, electron-electron exchange interaction and static dielectric susceptibility of model (1.1). In particular, it was established using Hubbard-I approximation that the interaction with local anharmonic vibrations (i.e. with pseudospin subsystem) leads to the splittings in electron spectrum and gives rise to the additional subbands. This influences the character of the electron states occupation and the behaviour of the chemical potential. By calculation of the occupation change under the influence of the transverse electric field (perpendicular to the CuO-layers in YBaCuO-type structures) the possibility of large values of static dielectric permeability for the case of partial filling of electron subbands was established [9].

Detailed study of dielectric and dynamic properties of pseudospin-electron model is important in the problem of possible connection between superconductivity and lattice instability of ferro- or antiferroelectric type in HTSC compounds [10-13]. The purpose of this paper is to obtain the expressions for Green functions and correlation functions determining the dielectric susceptibility and giving information about the spectrum of low-frequency vibrations and to evaluate, on this basis, so-called "transverse" dielectric susceptibility for certain values of electron concentration n ($0 < n < 1$), asymmetry parameter h and chemical potential μ [14,15].

2 Hamiltonian and initial relations

We shall write the Hamiltonian and the operators corresponding to physical quantities in the second quantized representation using the Hubbard operators X_i^{pq}, acting in the space of eight states $|R\rangle = |n_{i\uparrow}, n_{i\downarrow}, S_i^z\rangle$ of the unit cell

$$\begin{aligned}
|1\rangle &= \left|0,0,\tfrac{1}{2}\right\rangle & |\tilde{1}\rangle &= \left|0,0,-\tfrac{1}{2}\right\rangle \\
|2\rangle &= \left|1,1,\tfrac{1}{2}\right\rangle & |\tilde{2}\rangle &= \left|1,1,-\tfrac{1}{2}\right\rangle \\
|3\rangle &= \left|0,1,\tfrac{1}{2}\right\rangle & |\tilde{3}\rangle &= \left|0,1,-\tfrac{1}{2}\right\rangle \\
|4\rangle &= \left|1,0,\tfrac{1}{2}\right\rangle & |\tilde{4}\rangle &= \left|1,0,-\tfrac{1}{2}\right\rangle .
\end{aligned} \tag{2.1}$$

In particular,

$$\begin{aligned}
a_{i\uparrow} &= X_i^{14} + X_i^{32} + X_i^{\tilde{1}\tilde{4}} + X_i^{\tilde{3}\tilde{2}}, & a_{i\downarrow} &= X_i^{13} - X_i^{42} + X_i^{\tilde{1}\tilde{3}} - X_i^{\tilde{4}\tilde{2}}, \\
n_{i\uparrow} &= X_i^{44} + X_i^{22} + X_i^{\tilde{4}\tilde{4}} + X_i^{\tilde{2}\tilde{2}}, & n_{i\downarrow} &= X_i^{33} + X_i^{22} + X_i^{\tilde{3}\tilde{3}} + X_i^{\tilde{2}\tilde{2}}, \\
S_i^z &= \frac{1}{2}\sum_{r=1}^{4}\left(X_i^{rr} - X_i^{\tilde{r}\tilde{r}}\right).
\end{aligned} \tag{2.2}$$

Then

$$H_i = \sum_{r=1}^{\tilde{4}} \lambda_r X_i^{rr} - \frac{\Omega}{2}\sum_{r=1}^{4}\left(X_i^{r\tilde{r}} + X_i^{\tilde{r}r}\right), \tag{2.3}$$

where

$$\lambda_{1,\tilde{1}} = \mp\frac{h}{2}, \quad \lambda_{2,\tilde{2}} = 2E_0 + U \pm g \mp \frac{h}{2}, \quad \lambda_{3,\tilde{3}} = \lambda_{4,\tilde{4}} = E_0 \pm \frac{1}{2}(g-h) \tag{2.4}$$

are the energies of single–site states.

The aim of the paper is to calculate Green functions

$$\begin{aligned} K_{lm}^{SS}(\tau-\tau') &= \left\langle T\tilde{S}_l^z(\tau)\tilde{S}_m^z(\tau')\right\rangle, \\ K_{lm}^{Sn}(\tau-\tau') &= \left\langle T\tilde{S}_l^z(\tau)\tilde{n}_m(\tau')\right\rangle, \\ K_{lm}^{nn}(\tau-\tau') &= \langle T\tilde{n}_l(\tau)\tilde{n}_m(\tau')\rangle \end{aligned} \tag{2.5}$$

constructed of the operators given in Heisenberg representation with imaginary time argument

$$\tilde{A}(\tau) = \mathrm{e}^{\tau H} A \mathrm{e}^{-\tau H}. \tag{2.6}$$

The dielectric susceptibility of the system is expressed in terms of the Fourier transforms of functions (2.5) using expansion in even Matsubara's frequencies (see below). The perturbation theory and diagram technique for Hubbard operators will be used to calculate these functions. Here we shall restrict ourselves to the case of absence of tunneling splitting in anharmonic potential well ($\Omega = 0$). Accordingly, the initial Hamiltonian can be rewritten as a sum

$$H = H_0 + H_{\text{int}}, \qquad H_0 = \sum_i \sum_{r=1}^{\tilde{4}} \lambda_r X_i^{rr}, \tag{2.7}$$

$$\begin{aligned} H_{\text{int}} = & \sum_{ij\sigma} t_{ij} \left(X_i^{41} + X_i^{23} + X_i^{\tilde{4}\tilde{1}} + X_i^{\tilde{2}\tilde{3}}\right)\left(X_j^{14} + X_j^{32} + X_j^{\tilde{1}\tilde{4}} + X_j^{\tilde{3}\tilde{2}}\right) + \\ & \sum_{ij\sigma} t_{ij} \left(X_i^{31} - X_i^{24} + X_i^{\tilde{3}\tilde{1}} - X_i^{\tilde{2}\tilde{4}}\right)\left(X_j^{13} - X_j^{42} + X_j^{\tilde{1}\tilde{3}} - X_j^{\tilde{4}\tilde{2}}\right). \end{aligned}$$

We shall use the standard representation of the $\exp(-\beta H)$ operator in the form

$$\mathrm{e}^{-\beta H} = \mathrm{e}^{-\beta H_0}\hat{\sigma}(\beta), \qquad \hat{\sigma}(\beta) = T\exp\left\{-\int_0^\beta H_{\text{int}}(\tau)d\tau\right\}. \tag{2.8}$$

Then we obtain for the functions $\left\langle T\tilde{X}_l^{pp}(\tau)\tilde{X}_m^{qq}(\tau')\right\rangle$, in terms of which the Green functions (2.5) are expressed, the following expressions

$$\begin{aligned} &\left\langle T\tilde{X}_l^{pp}(\tau)\tilde{X}_m^{qq}(\tau')\right\rangle \equiv K_{lm}^{(pq)}(\tau-\tau') = \\ &\frac{1}{\langle\hat{\sigma}(\beta)\rangle_0}\langle TX_l^{pp}(\tau)X_m^{qq}(\tau')\hat{\sigma}(\beta)\rangle_0 = \langle TX_l^{pp}(\tau)X_m^{qq}(\tau')\hat{\sigma}(\beta)\rangle_0^c. \end{aligned} \tag{2.9}$$

Here, the operators are given in the interaction representation

$$A(\tau) = \mathrm{e}^{\tau H_0} A \mathrm{e}^{-\tau H_0}; \tag{2.10}$$

the averaging $\langle\ldots\rangle_0$ is performed over the statistical distribution with Hamiltonian H_0, and symbol $\langle\ldots\rangle_0^c$ denotes the separation of connected diagrams (that is, the diagrams which do not split in the isolated parts without external vertices while cutting of interaction lines t_{ij}).

3 Perturbation theory for Green functions and diagram technique

Expansion of the exponent in (2.8) in powers of H_{int} leads, after substitution in eq. (2.9), to the expression that has the form of the sum of infinite series with the terms presented by the averages of T–products of Hubbard operators in interaction representation. The evaluation of such averages can be performed using Wick's theorem for Hubbard operators [14,15]. This theorem gives the algorithm reducing the average of product of n X–operators to the sum of averages of products of $n-1$ X–operators. Finally, this gives the possibility to express result in terms of the products of nonperturbated Green functions $g_{ij}^{pq}(\tau-\tau')=\delta_{ij}g^{pq}(\tau-\tau')$, where

$$g^{pq}(\tau-\tau')=\frac{\langle TX^{pq}(\tau)X^{qp}(\tau')\rangle_0}{\left\langle [X^{pq},X^{qp}]_{\pm}\right\rangle_0}=\mathrm{e}^{(\tau-\tau')\lambda_{pq}}\begin{cases}\pm n_{\pm}\left(\lambda_{pq}\right) & ,\tau>\tau' \\ \pm n_{\pm}\left(\lambda_{pq}\right)-1 & ,\tau<\tau'\end{cases},$$

$$n_{\pm}\left(\lambda_{pq}\right)=\frac{1}{\mathrm{e}^{\beta\lambda_{pq}}\pm 1},\qquad \lambda_{pq}=\lambda_p-\lambda_q \tag{3.1}$$

and averages of certain number of the diagonal X–operators (in expression (3.1) "+" sign refers to the case when both X–operators are of Fermi type, otherwise the "−" sign applies). The averages of the products of diagonal operators are in turn expanded in semi–invariants

$$\langle X_i^{pp}\rangle_0=b_p,\qquad \left\langle X_i^{pp}X_j^{qq}\right\rangle_0=b_{pq}\delta_{ij}+b_pb_q, \tag{3.2}$$

$$\left\langle X_i^{pp}X_j^{qq}X_l^{rr}\right\rangle_0=b_{pqr}\delta_{ij}\delta_{il}+b_{pq}\delta_{ij}b_r+b_{pr}\delta_{il}b_q+b_{qr}\delta_{jl}b_p+b_pb_qb_r,$$

etc., where

$$\begin{aligned} b_p &= \langle X^{pp}\rangle_0=\mathrm{e}^{-\beta\lambda_p}\left[\sum_s \mathrm{e}^{-\beta\lambda_s}\right]^{-1}, \\ b_{pq} &= \langle X^{pp}X^{qq}\rangle_{0c}=\frac{\partial}{\partial\left(-\beta\lambda_p\right)}b_q=\frac{\partial}{\partial\left(-\beta\lambda_q\right)}b_p, \\ b_{pqr} &= \langle X^{pp}X^{qq}X^{rr}\rangle_{0c}=\frac{\partial^2}{\partial\left(-\beta\lambda_p\right)\partial\left(-\beta\lambda_q\right)}b_r. \end{aligned} \tag{3.3}$$

Let us demonstrate the above described procedure for the case of evaluation of $\left\langle T\tilde{X}_l^{11}(\tau)\tilde{X}_m^{11}(\tau')\right\rangle$, separating one of the terms which appear in the second order of the perturbation theory

$$\int\limits_0^\beta d\tau_1\int\limits_0^\beta d\tau_2\sum_{iji_1j_1}t_{ij}t_{i_1j_1}\left\langle TX_l^{11}(\tau)X_m^{11}(\tau')X_i^{41}(\tau_1)X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0. \tag{3.4}$$

The stepwise pairing of certain nondiagonal operator with the other ones gives the possibility to reduce expression (3.4) to the sum of averages of the smaller number of operators

$$\left\langle TX_l^{11}(\tau)X_m^{11}(\tau')X_i^{41}(\tau_1)X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0=$$

$$\left\langle T\, \overleftarrow{X_l^{11}(\tau)X_m^{11}(\tau')X_i^{41}}(\tau_1)X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0 +$$

$$\left\langle TX_l^{11}(\tau)\, \overleftarrow{X_m^{11}(\tau')X_i^{41}}(\tau_1)X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0 +$$

$$\left\langle TX_l^{11}(\tau)X_m^{11}(\tau')\, \overrightarrow{X_i^{41}(\tau_1)X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}}(\tau_2)\right\rangle_0 = \tag{3.5}$$

$$g_{il}^{41}(\tau_1-\tau)\left\langle TX_l^{41}(\tau)X_m^{11}(\tau')X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0 +$$

$$g_{im}^{41}(\tau_1-\tau')\left\langle TX_l^{11}(\tau)X_m^{41}(\tau')X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)X_{j_1}^{14}(\tau_2)\right\rangle_0 +$$

$$g_{ij_1}^{41}(\tau_1-\tau_2)\left\langle TX_l^{11}(\tau)X_m^{11}(\tau')X_j^{14}(\tau_1)X_{i_1}^{41}(\tau_2)\left(X_{j_1}^{11}+X_{j_1}^{44}\right)^{\tau_2}\right\rangle_0 .$$

We use the following priority rule for X–operators in the pairing procedure: $X^{41} > X^{31} > X^{43}$; $X^{23} > X^{24} > X^{34}$ (see, [15]). The successive applications of pairing procedure for (3.5) lead, finally, to

$$(3.4) = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{ij} t_{ij} \sum_{i_1 j_1} t_{i_1 j_1}$$

$$\Big\{ g_{il}^{41}(\tau_1-\tau)g_{i_1m}^{41}(\tau_2-\tau')g_{lj_1}^{41}(\tau-\tau_2)g_{mj}^{41}(\tau'-\tau_1)\times \tag{3.6a}$$

$$\left\langle T\left(X_j^{11}+X_j^{44}\right)^{\tau_1}\left(X_{j_1}^{11}+X_{j_1}^{44}\right)^{\tau_2}\right\rangle_0 + [(i,j,\tau_1)\rightleftharpoons(i_1,j_1,\tau_2)] +$$

$$g_{il}^{41}(\tau_1-\tau)g_{i_1j}^{41}(\tau_2-\tau_1)g_{lm}^{41}(\tau-\tau')g_{mj_1}^{41}(\tau'-\tau_2)\times \tag{3.6b}$$

$$\left\langle T\left(X_j^{11}+X_j^{44}\right)^{\tau_1}\left(X_{j_1}^{11}+X_{j_1}^{44}\right)^{\tau_2}\right\rangle_0 + [(i,j,\tau_1)\rightleftharpoons(i_1,j_1,\tau_2)] +$$

$$[(l,\tau)\rightleftharpoons(m,\tau')] + \left[\begin{matrix}(i,j,\tau_1)\\(l,\tau)\end{matrix} \rightleftharpoons \begin{matrix}(i_1,j_1,\tau_2)\\(m,\tau')\end{matrix}\right] +$$

$$g_{il}^{41}(\tau_1-\tau)g_{i_1j}^{41}(\tau_2-\tau_1)g_{lj_1}^{41}(\tau-\tau_2)\times$$

$$\left\langle TX_m^{11}(\tau')\left(X_j^{11}+X_j^{44}\right)^{\tau_1}\left(X_{j_1}^{11}+X_{j_1}^{44}\right)^{\tau_2}\right\rangle_0 + \tag{3.6c}$$

$$[(i,j,\tau_1)\rightleftharpoons(i_1,j_1,\tau_2)] + [(l,\tau)\rightleftharpoons(m,\tau')] +$$

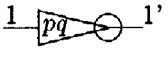
$$\left[\begin{matrix}(i,j,\tau_1)\\(l,\tau)\end{matrix} \rightleftharpoons \begin{matrix}(i_1,j_1,\tau_2)\\(m,\tau')\end{matrix}\right] + g_{ij_1}^{41}(\tau_1-\tau_2)g_{i_1j}^{41}(\tau_2-\tau_1)\times$$

$$\left\langle TX_l^{11}(\tau)X_m^{11}(\tau')\left(X_j^{11}+X_j^{44}\right)^{\tau_1}\left(X_{j_1}^{11}+X_{j_1}^{44}\right)^{\tau_2}\right\rangle_0 \Big\}. \tag{3.6d}$$

We introduce the diagrammatic notations

• ; ⓟⓟ – free vertex; diagonal operator,

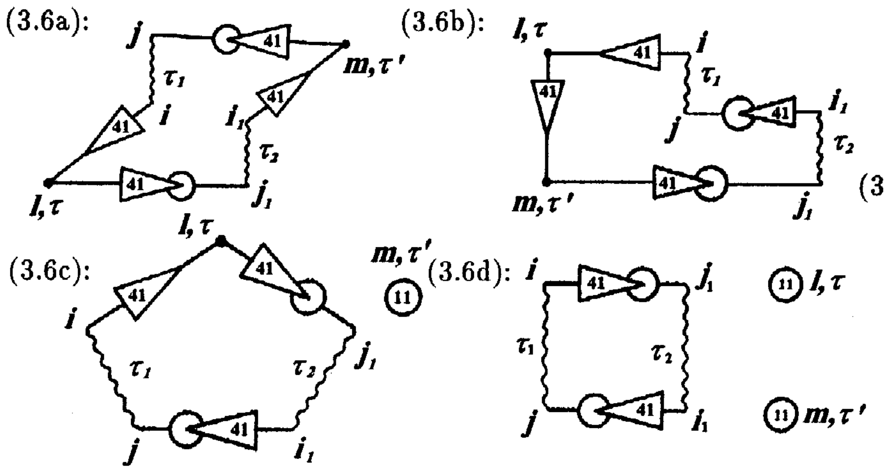
– $g_{11'}^{pq}(\tau_1-\tau_1')$,



– $g_{11'}^{pq}(\tau_1-\tau_1')\left(X_{1'}^{pp}+X_{1'}^{qq}\right)$,

– $t_{11'}$ (3.7)

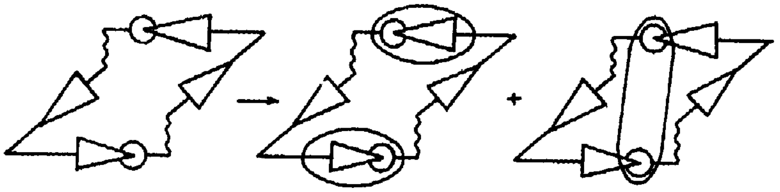
The diagrams



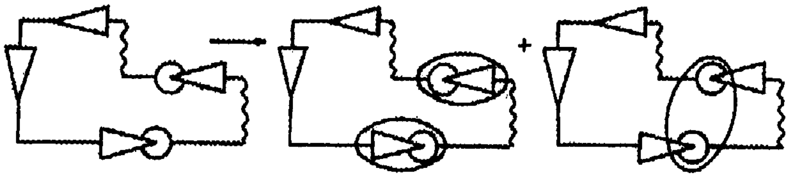
(3.8)

correspond to the expression (3.6) (with additional diagrams obtained from (3.8) by corresponding permutations)

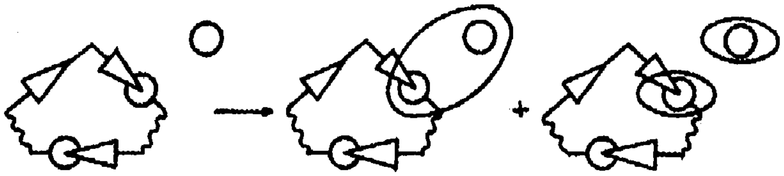
The expansion of (3.6) in semi–invariants leads to the multiplication of diagrams (semi–invariants are represented by ovals surrounding corresponding vertices with diagonal operators). For example,



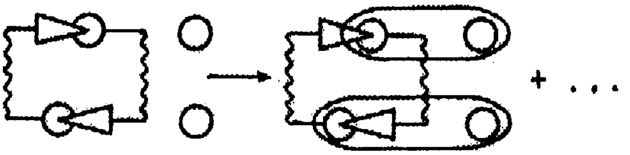
(3.9a)



(3.9b)



(3.9c)



(3.9d)

The diagrams of the same form appear in the other contributions of the second order in t_{ij} entering average $\left\langle T\tilde{X}_l^{11}(\tau)\tilde{X}_m^{11}(\tau')\right\rangle$. However, the additional diagrams containing lines corresponding to Green functions constructed of spin flipping operators X^{34} or $X^{\tilde{3}\tilde{4}}$ (which are Bose–type operators) can appear (e.g., evaluating $\langle TX_l^{11}X_m^{11}X_i^{41}X_j^{14}X_{i_1}^{31}X_{j_1}^{13}\rangle)$. These diagrams are important for evaluation of the magnetic susceptibility (see, [18]).

Let us proceed to the momentum–frequency representation in the expressions for Green functions as well as in their diagrammatic representations. The following notations are introduced

$$\int_0^\beta d(\tau-\tau')e^{-i\bar{\omega}_n(\tau-\tau')}\frac{1}{N}\sum_{lm}K_{lm}^{(pr)}(\tau-\tau')e^{i\mathbf{q}(\mathbf{R}_l-\mathbf{R}_m)} = K^{(pr)}(\mathbf{q},\bar{\omega}_n). \quad (3.10)$$

The nonperturbative Green functions are expanded into series

$$g^{pq}(\tau) = \frac{1}{\beta}\sum_n e^{i\omega_n\tau}g^{pq}(\omega_n),$$
$$g^{pq}(\omega_n) = \frac{1}{i\omega_n - \lambda_{pq}}; \qquad \omega_n = \frac{2n+1}{\beta}\pi \quad (3.11)$$

for Fermi–type functions, and

$$g^{rs}(\tau) = \frac{1}{\beta}\sum_n e^{i\bar{\omega}_n\tau}g^{rs}(\bar{\omega}_n),$$
$$g^{rs}(\bar{\omega}_n) = -\frac{1}{i\bar{\omega}_n - \lambda_{rs}}; \qquad \bar{\omega}_n = \frac{2n}{\beta}\pi \quad (3.12)$$

for Bose–type functions.

Integration over time variables $(\tau_1,\dots,\tau_n)$ in the expressions corresponding to diagrams leads to the conservation law type conditions for the frequencies at each diagram vertex due to the relation

$$\int_0^\beta e^{i(\sum\omega_n)\tau}d\tau = \beta\delta\left(\sum\omega_n\right) \quad (3.13)$$

(after Fourier transformation, the same holds for the wave vectors).

For example, performing transformation (3.10) we obtain the following expressions for some of diagrams (3.9)

$$(3.9a)_I \quad : \quad -\frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1}t_{\mathbf{k}_1}g_{\mathbf{k}_1}^{41}(\omega_{n_1})\,g_{\mathbf{q}+\mathbf{k}_1}^{41}(\bar{\omega}_n-\omega_{n_1})\times$$
$$t_{\mathbf{q}+\mathbf{k}_1}g_{\mathbf{q}+\mathbf{k}_1}^{41}(\bar{\omega}_n+\omega_{n_1})\,g_{\mathbf{k}_1}^{41}(\omega_{n_1})\left\langle X^{11}+X^{44}\right\rangle_0^2, \quad (3.14a)$$

$$(3.9b)_I \quad : \quad -\frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1}t_{\mathbf{k}_1}^2\left[g_{\mathbf{k}_1}^{41}(\omega_{n_1})\left\langle X^{11}+X^{44}\right\rangle_0\right]^2\times$$
$$g_{\mathbf{k}_1}^{41}(\omega_{n_1})\,g_{\mathbf{q}+\mathbf{k}_1}^{41}(\bar{\omega}_n+\omega_{n_1}), \quad (3.14b)$$

$$(3.9c)_I \; : \; -\delta(\bar{\omega}_n)\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} t^2_{\mathbf{k}_1} g^{41}_{\mathbf{k}_1}(\omega_{n_1})\left\langle X^{11}+X^{44}\right\rangle_0 \times$$

$$g^{41}_{\mathbf{k}_1}(\omega_{n_1})\, g^{41}_{\mathbf{q}+\mathbf{k}_1}(\omega_{n_1})\left\langle X^{11}\left(X^{11}+X^{44}\right)\right\rangle_{0c}, \qquad (3.14c)$$

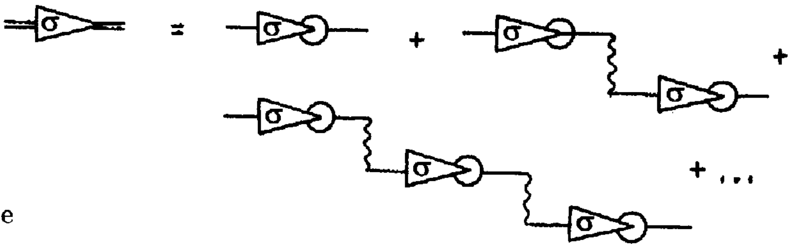
$$(3.9d)_I \; : \; -\beta\delta(\bar{\omega}_n)\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} t_{\mathbf{k}_1} t_{\mathbf{q}+\mathbf{k}_1} g^{41}_{\mathbf{k}_1}(\omega_{n_1})\, g^{41}_{\mathbf{q}+\mathbf{k}_1}(\omega_{n_1}) \times$$

$$\left\langle X^{11}\left(X^{11}+X^{44}\right)\right\rangle_{0c}\left\langle X^{11}\left(X^{11}+X^{44}\right)\right\rangle_{0c}. \qquad (3.14d)$$

Here, $t_{\mathbf{k}}$, $g^{pq}_{\mathbf{k}}$ are Fourier transforms of transfer integral t_{ij} and function g^{pq}_{ij}, respectively (for nonperturbed function $g^{pq}_{\mathbf{k}} \equiv g^{pq}$).

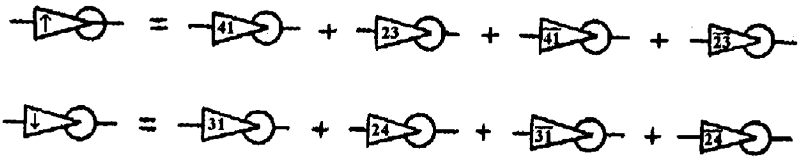
4 Diagrammatic series for Green function with diagonal X–operators

The distinct feature of already presented diagrams and of the diagrams corresponding to the other orders of perturbation theory is the presence of chain fragments (i.e. ones where links are connected by wavy lines t_{ij}). The simplest series of chain diagrams



(4.1)

where



(4.2)

corresponds, as in the case of ordinary Hubbard model (see, [15]), to Hubbard–I approximation for single–electron Green functions. The expressions

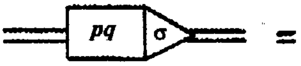
$$\mathcal{G}^{\sigma}_{\mathbf{k}}(\omega_n) = \frac{1}{g^{-1}_{\sigma}(\omega_n) - t_{\mathbf{k}}}, \qquad (4.3)$$

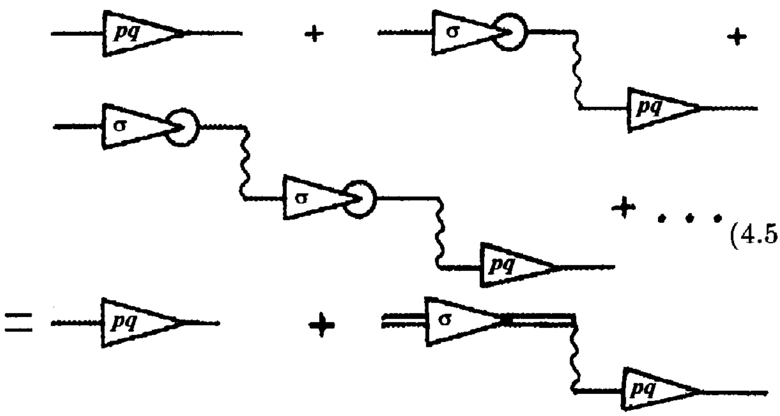
$$\begin{aligned} g_{\uparrow}(\omega_n) &= \frac{\langle X^{11}+X^{44}\rangle}{i\omega_n-\lambda_{41}} + \frac{\langle X^{22}+X^{33}\rangle}{i\omega_n-\lambda_{23}} + \\ &\quad \frac{\left\langle X^{\tilde{1}\tilde{1}}+X^{\tilde{4}\tilde{4}}\right\rangle}{i\omega_n-\lambda_{\tilde{4}\tilde{1}}} + \frac{\left\langle X^{\tilde{2}\tilde{2}}+X^{\tilde{3}\tilde{3}}\right\rangle}{i\omega_n-\lambda_{\tilde{2}\tilde{3}}}, \\ g_{\downarrow}(\omega_n) &= \frac{\langle X^{11}+X^{33}\rangle}{i\omega_n-\lambda_{31}} + \frac{\langle X^{22}+X^{44}\rangle}{i\omega_n-\lambda_{24}} + \\ &\quad \frac{\left\langle X^{\tilde{1}\tilde{1}}+X^{\tilde{3}\tilde{3}}\right\rangle}{i\omega_n-\lambda_{\tilde{3}\tilde{1}}} + \frac{\left\langle X^{\tilde{2}\tilde{2}}+X^{\tilde{4}\tilde{4}}\right\rangle}{i\omega_n-\lambda_{\tilde{2}\tilde{4}}} \end{aligned} \qquad (4.4)$$

correspond to the graphs (4.1), (4.2) in momentum–frequency representation. The poles of function $\mathcal{G}^{\sigma}_{\mathbf{k}}(\omega_n)$ determine the spectrum of single–electron excitations. This spectrum was investigated in detail in [7]. One of its main features is the presence of additional subbands in comparison with Hubbard model (in addition to subbands (41), (31), (23) and (24) there appear $(\tilde{4}\tilde{1})$, $(\tilde{3}\tilde{1})$, $(\tilde{2}\tilde{3})$ and $(\tilde{2}\tilde{4})$ ones; the difference between the first group and the second one is connected with different pseudospin orientation at single–electron transition).

For the case, when the chain in diagram starts or terminates in the external vertex, the corresponding nearest Green function is determined by operator index of this vertex. The following notations are used for such series

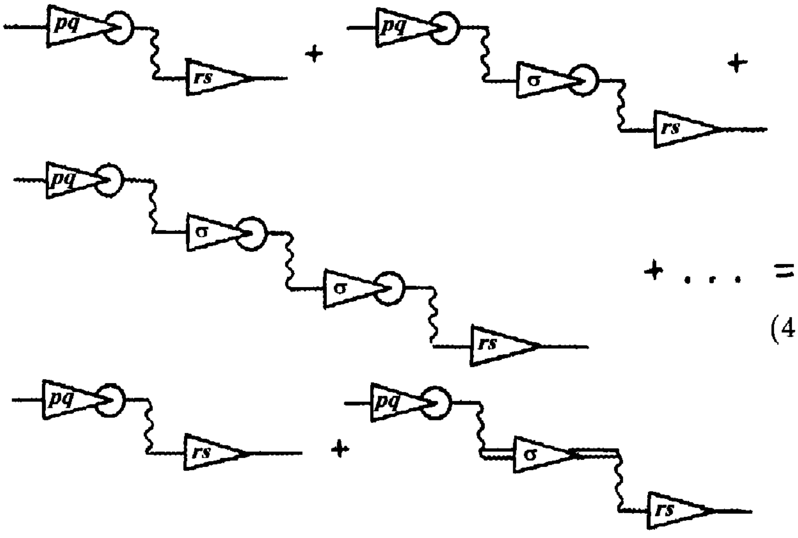
$\Gamma^{\sigma}_{pq}(\mathbf{k},\omega_n) \equiv$





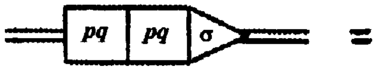
(4.5)

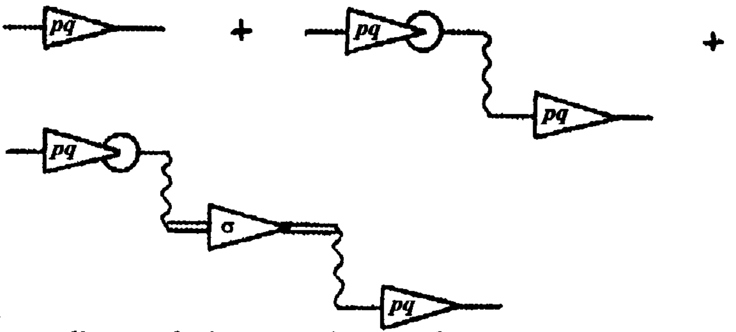
$\tilde{G}^{\sigma}_{pq,rs}(\mathbf{k},\omega_n) \equiv$



(4.6)

$G^{\sigma}_{pq,pq}(\mathbf{k},\omega_n) \equiv$





(4.7)

The corresponding analytic expressions read:

$$\begin{aligned}
\Gamma^{\sigma}_{pq}\left(\mathbf{k},\omega_n\right) &= \frac{g^{pq}\left(\omega_n\right)}{1-t_{\mathbf{k}}g\left(\omega_n\right)}, \\
\tilde{G}^{\sigma}_{pq,rs}\left(\mathbf{k},\omega_n\right) &= g^{pq}\left(\omega_n\right)t_{\mathbf{k}}g^{rs}\left(\omega_n\right)\frac{\left\langle X^{pp}+X^{qq}\right\rangle}{1-t_{\mathbf{k}}g\left(\omega_n\right)}, \qquad (4.8)\\
G^{\sigma}_{pq,pq}\left(\mathbf{k},\omega_n\right) &= g^{pq}\left(\omega_n\right)\left[1+t_{\mathbf{k}}g^{pq}\left(\omega_n\right)\frac{\left\langle X^{pp}+X^{qq}\right\rangle}{1-t_{\mathbf{k}}g\left(\omega_n\right)}\right].
\end{aligned}$$

Let us now return to the problem of diagram series for average $K^{(pq)}_{lm}(\tau-\tau')=\left\langle T\tilde{X}^{pp}_{l}(\tau)\tilde{X}^{qq}_{m}(\tau')\right\rangle$ taking into account the above mentioned arguments. It is convenient to write down this function in the form

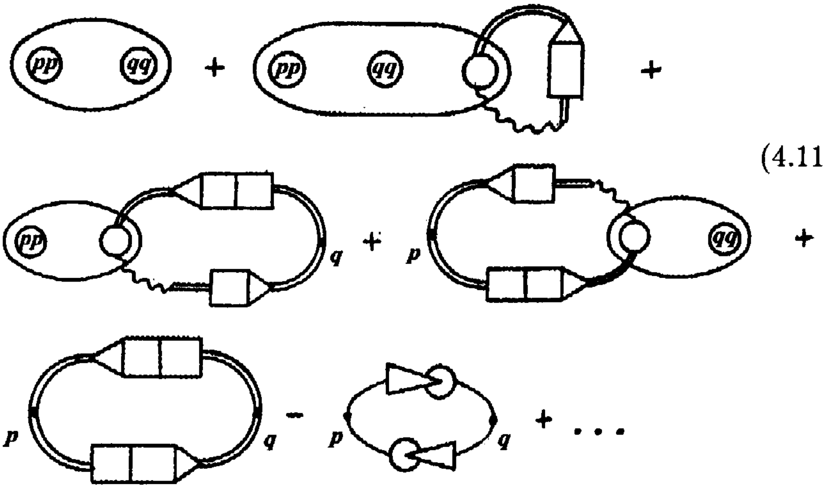
$$K^{(pq)}_{lm}(\tau-\tau')=\bar{K}^{(pq)}_{lm}(\tau-\tau')+\left\langle X^{pp}_{l}\right\rangle\left\langle X^{qq}_{m}\right\rangle, \qquad (4.9)$$

with the use of semi-invariant

$$\bar{K}^{(pq)}_{lm}(\tau-\tau')=\left\langle T\tilde{X}^{pp}_{l}(\tau)\tilde{X}^{qq}_{m}(\tau')\right\rangle_{c}. \qquad (4.10)$$

The diagram series, with the accepted priority rule, has the form

$\bar{K}^{pq} =$

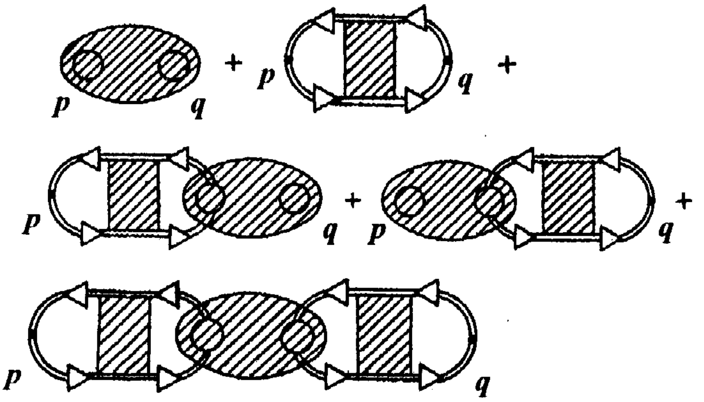


(4.11)

Here, the summation of chain fragments is performed. This enables one to pass to the propagator lines (4.5)–(4.7) [1].

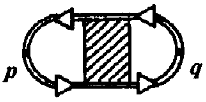
Analysis of structure of the diagram series for function $\bar{K}^{pq}$ can be performed in the same way [18,19]. The consideration of diagrams of higher order of perturbation theory leads to the conclusion that this function can be presented in the form

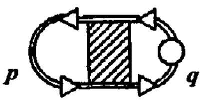
$\bar{K}^{pq} =$

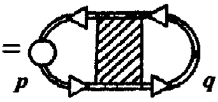


(4.12)

Each quantity in (4.12) is a (8×8)–matrix in space of single–site states $(p, q = 1, \ldots, 4, \tilde{1}, \ldots, \tilde{4})$. Quantities

$\Pi''_{pq} =$ 

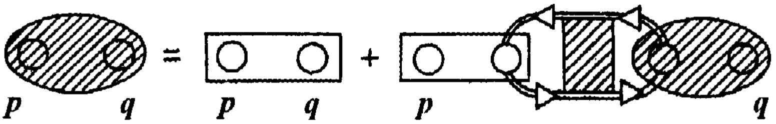
$'\Pi_{pq} =$ 

$\Pi'_{pq} =$ 

(4.13)

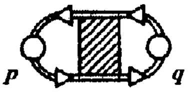
being sums of the diagrams in which one or both external vertices are free (are not included in the semi–invariant averages); diagrams entering (4.13) do not break into independent parts if any of the semi–invariants is cut.

The first term in (4.12) is the "full" semi–invariant of the second order $\bar{\bar{b}}_{pq}$, which satisfies the Dyson–type equation



(4.14)

Here  $= \tilde{b}_{pq}$ is the second–order semi–invariant renormalized due to the "single–tail" or "multi–tail" parts (one of the diagrams that give such contribution is shown in (4.11): diagram No 2);

$\Pi_{pq} =$ 

(4.15)

is the irreducible part (that can not be broken across ), both vertices of this diagram are to be averaged in semi–invariants together with vertices from the other parts of diagrams.

Solution of the equation (4.14) can be written as a matrix

$$\bar{\bar{b}} = \left(1 - \tilde{b}\Pi\right)^{-1} \tilde{b}. \qquad (4.16)$$

---

[1] The diagrams like the last one in (4.11) containing bare Green functions, contribute to renormalization of semi-invariants (see, [19]).

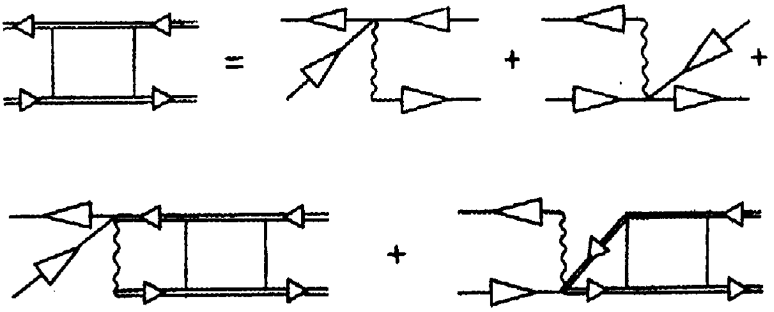
In the same way starting from (4.12), we can represent the correlator $\bar{K}^{pq}$ in the form

$$\bar{K} = \bar{\bar{\bar{b}}} + \Pi'' + {}'\Pi\bar{\bar{\bar{b}}} + \bar{\bar{\bar{b}}}\Pi' + {}'\Pi\bar{\bar{\bar{b}}}\Pi'. \tag{4.17}$$

Hence, the problem of calculation of this correlator reduces to the calculation of the irreducible parts (4.13), (4.15) and semi–invariants in any approximation.

5 Generalized Random Phase Approximation

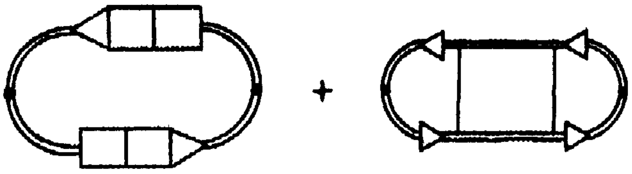
In the summation of diagrams entering functions (4.13), (4.15), we shall restrict ourselves to the contributions from the so-called ladder diagrams with antiparallel lines. This corresponds to the so-called generalized random phase approximation (GRPA) (which was applied in [18,19] where the magnetic susceptibility of the ordinary Hubbard model and $t-J$ model was considered). Diagram series for the functions (4.13), (4.15) appearing in this case can be obtained starting from the equation



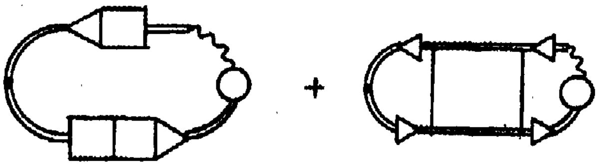
(5.1)

and then connecting the external lines on the left and right sides of the diagrams to the free vertices or to the vertices to be included into semi–invariants (in the last case this is performed with the help of additional wavy line). Then

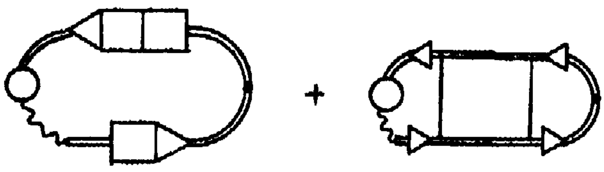
$\Pi''_{pq} =$



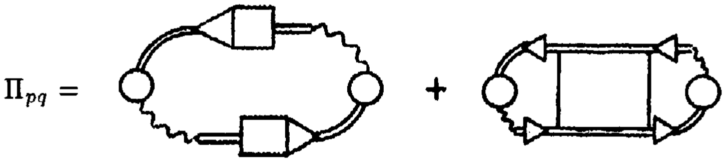
${}'\Pi_{pq} =$



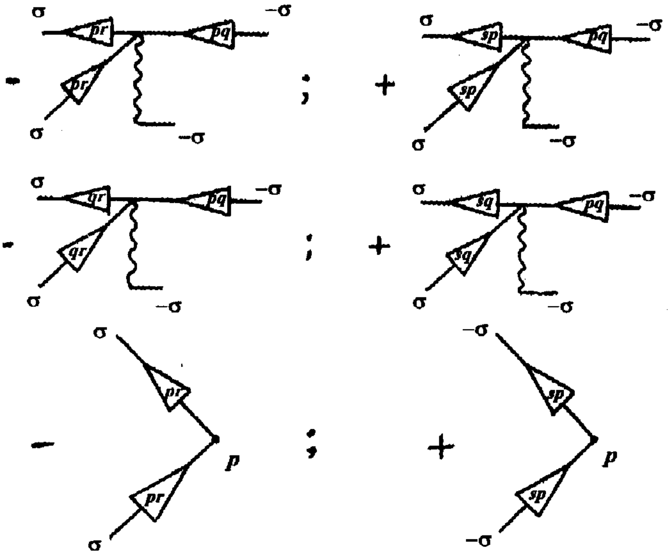
$\Pi'_{pq} =$



(5.2)



For given p and q, the existence of nonzero contributions in (5.2) and their signs are determined by selection rules following from the consideration of elementary vertices of diagrams. For example,



(5.3)

Multiplication of diagrams (5.2) according to (5.1), leads to the appearance of multi–loop diagrams. Neighbouring loops appearing in this case contain Green function corresponding to the opposite spin directions. Spin is conserved along separate chain in the loop. Pairings which can lead to the spin flipping are accompanied by appearance of operators X^{34} (or $X^{\bar{3}\bar{4}}$). This, in turn, gives rise to boson functions g^{34}, $g^{\bar{3}\bar{4}}$. Such scattering processes are neglected in approximation (5.1).

Multi–loop diagrams contain the zero order loops as elements in the right hand parts of the relations (5.2). We introduce the shortened notations for them

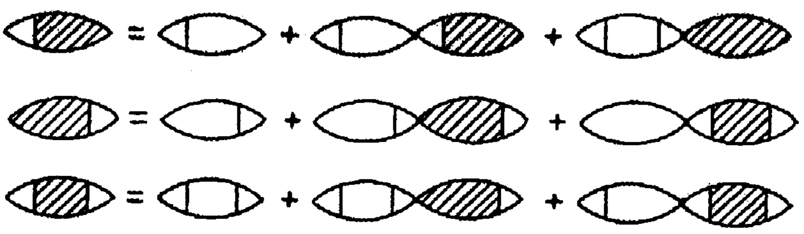
(5.4)

and

(5.5)

for renormalized loops, respectively.

The summation of the series appearing due to multiplication of diagrams (5.2) leads to the set of equations for loops (5.5)



(5.6)

Elements of these graphs are matrices with respect to p, q and spin indices. Circles • correspond to the matrices $\gamma^{\sigma\sigma'}_{pp'} = \delta_{pp'}\delta_{\sigma,-\sigma'}$. Matrices (5.4) contain factors $\delta_{\sigma\sigma'}$. Equations of the set (5.6) are written in the explicit form as

$$\Pi''^{,\sigma\sigma'}_{pp'} = \Pi''^{,\sigma}_{(0)pp'}\delta_{\sigma\sigma'} + \sum_{p_1=1}^{4} \Pi''^{,\sigma}_{(0)pp_1}\Pi'^{,-\sigma\sigma'}_{p_1p'} + \sum_{\tilde{p}_1=1}^{4} \Pi''^{,\sigma}_{(0)p\tilde{p}_1}\Pi'^{,-\sigma\sigma'}_{\tilde{p}_1p'} + \sum_{p_1=1}^{4} {}'\Pi^{\sigma}_{(0)p\dot{p}_1}\Pi''^{,-\sigma\sigma'}_{p_1p'} + \sum_{\tilde{p}_1=1}^{4} {}'\Pi^{\sigma}_{(0)p\tilde{p}_1}\Pi''^{,-\sigma\sigma'}_{\tilde{p}_1p'}, \tag{5.7}$$

$$\Pi'^{,\sigma\sigma'}_{pp'} = \Pi'^{,\sigma}_{(0)pp'}\delta_{\sigma\sigma'} + \sum_{p_1=1}^{4} \Pi'^{,\sigma}_{(0)pp_1}\Pi'^{,-\sigma\sigma'}_{p_1p'} + \sum_{\tilde{p}_1=1}^{4} \Pi'^{,\sigma}_{(0)p\tilde{p}_1}\Pi'^{,-\sigma\sigma'}_{\tilde{p}_1p'} + \sum_{p_1=1}^{4} \Pi^{\sigma}_{(0)pp_1}\Pi''^{,-\sigma\sigma'}_{p_1p'} + \sum_{\tilde{p}_1=1}^{4} \Pi^{\sigma}_{(0)p\tilde{p}_1}\Pi''^{,-\sigma\sigma'}_{\tilde{p}_1p'}.$$

The other two equations are written in the similar way.

Overall contributions to the irreducible parts (5.2) are formed by summed over spin indices solutions of above set of equations:

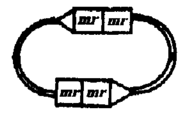
$$\Pi''_{pp'} = \sum_{\sigma,\sigma'} \Pi''^{,\sigma\sigma'}_{pp'}, \text{ etc.} \tag{5.8}$$

6 Elementary loop diagrams (zero–order loops)

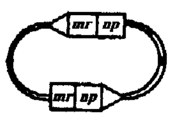
Our next aim is to obtain explicit expressions for polarization loops of the zero–order approximation (5.4).

Matrix $\Pi''_{(0)pq}$. There are loops of two types among the diagrams corresponding to matrix $\Pi''_{(0)}$:

$\Phi''(mr) =$



$\Psi''(mr, np) =$



(6.1)

where $((mr) \neq (np))$. Analytical expressions for them can be obtained starting from formulas (4.6)–(4.8)

$$\Phi''(mr) = \frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} G^{\sigma}_{mr,mr}(\mathbf{k}_1,\omega_{n_1})\, G^{\sigma}_{mr,mr}(\mathbf{q}+\mathbf{k}_1,\bar{\omega}_n+\omega_{n_1}), \tag{6.2}$$

$$\Psi''(mr,np) = \frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} \tilde{G}^{\sigma}_{mr,np}(\mathbf{k}_1,\omega_{n_1})\, \tilde{G}^{\sigma}_{np,mr}(\mathbf{q}+\mathbf{k}_1,\bar{\omega}_n+\omega_{n_1}).$$

Functions G or $\tilde{G}$ have poles coinciding with those of electron Green functions $\mathcal{G}_k^\sigma(\omega_n)$ and defining single–electron spectrum $\varepsilon_\alpha(\mathbf{k})$ of the model. Using decomposition in simple fractions

$$\tilde{G}^\sigma_{mr,np}(\mathbf{k}_1,\omega_{n_1}) = \sum_\alpha \frac{\tilde{A}^\alpha_{mr,np}(\mathbf{k}_1)}{i\omega_{n_1}-\varepsilon_\alpha(\mathbf{k}_1)}, \quad G^\sigma_{mr,mr}(\mathbf{k}_1,\omega_{n_1}) = \sum_\alpha \frac{A^\alpha_{mr,mr}(\mathbf{k}_1)}{i\omega_{n_1}-\varepsilon_\alpha(\mathbf{k}_1)}, \tag{6.3}$$

we obtain

$$\begin{aligned} \Phi''(mr) \quad = \quad & \frac{1}{N}\sum_{\mathbf{k}_1}\sum_{\alpha\beta} A^\alpha_{mr,mr}(\mathbf{k}_1)\, A^\beta_{mr,mr}(\mathbf{q}+\mathbf{k}_1) \times \\ & \frac{n_+\left[\varepsilon_\alpha(\mathbf{k}_1)\right] - n_+\left[\varepsilon_\alpha(\mathbf{q}+\mathbf{k}_1)\right]}{i\bar{\omega}_n + \varepsilon_\alpha(\mathbf{k}_1) - \varepsilon_\alpha(\mathbf{q}+\mathbf{k}_1)} \end{aligned} \tag{6.4}$$

and the similar expression for $\Psi''(mr,np)$. The following relation is used in order to perform summation over frequency:

$$\frac{1}{\beta}\sum_{n_1} \frac{1}{i\omega_{n_1}-\lambda_1}\cdot\frac{1}{i\omega_{n_1}+i\bar{\omega}_n-\lambda_2} = \frac{n_+(\lambda_1)-n_+(\lambda_2)}{i\bar{\omega}_n+\lambda_1-\lambda_2}. \tag{6.5}$$

This relation follows from the definition of Fourier transform of nonperturbated Fermi–type Green function (see also, [15]).

Expressions of (6.4) type contain contributions both from intraband ($\alpha = \beta$) and interband ($\alpha \neq \beta$) transitions. For $T \to 0$ the first ones arise from the partially filled subband (with chemical potential inside); interband transitions take place between occupied and unoccupied states of different subbands.

Substantial simplifications are achieved for the case of independent subband approximation (corresponding to the situation when subbands widths are small in comparison with the distance between them: $t \ll U, t \ll g$). Then,

$$\begin{aligned} G^\sigma_{pq,pq}(\mathbf{k},\omega_n) \quad &\approx \quad \frac{1}{i\omega_n - \varepsilon_{pq}(\mathbf{k})}, \\ \tilde{G}^\sigma_{pq,rs}(\mathbf{k},\omega_n) \quad &\approx \quad \frac{t_\mathbf{k} B_{pq}}{\varepsilon_{pq}(\mathbf{k}) - \varepsilon_{rs}(\mathbf{k})}\left(\frac{1}{i\omega_n-\varepsilon_{pq}(\mathbf{k})} - \frac{1}{i\omega_n-\varepsilon_{rs}(\mathbf{k})}\right) \end{aligned} \tag{6.6}$$

and

$$\Phi''(mr) = \frac{1}{N}\sum_\mathbf{k} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{mr}(\mathbf{q}+\mathbf{k})\right]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{q}+\mathbf{k})}, \tag{6.7}$$

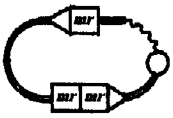
$$\begin{aligned} \Psi''(mr,np) = \frac{1}{N}\sum_\mathbf{k} \frac{B_{mr}B_{np}t_\mathbf{k}t_{\mathbf{k}+\mathbf{q}}}{\varepsilon_{mr}(\mathbf{k})-\varepsilon_{np}(\mathbf{k})}\cdot\frac{1}{\varepsilon_{mr}(\mathbf{k}+\mathbf{q})-\varepsilon_{np}(\mathbf{k}+\mathbf{q})} \times \\ \left[\frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right]-n_+\left[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n+\varepsilon_{mr}(\mathbf{k})-\varepsilon_{mr}(\mathbf{k}+\mathbf{q})} + \frac{n_+\left[\varepsilon_{np}(\mathbf{k})\right]-n_+\left[\varepsilon_{np}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n+\varepsilon_{np}(\mathbf{k})-\varepsilon_{np}(\mathbf{k}+\mathbf{q})}\right], \end{aligned}$$

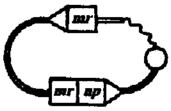
respectively. Here we neglect the contributions corresponding to the interband (mr) to (np) transitions. Here

$$\varepsilon_{pq}(\mathbf{k}) = \lambda_{pq} + B_{pq}t_\mathbf{k}; \qquad B_{pq} = \langle X^{pp} + X^{qq}\rangle \tag{6.8}$$

are the energies of separate noninteracting subbands.

Matrices $'\Pi_{(0)pq}, \Pi'_{(0)pq}$. The diagrams for the matrices $'\Pi_{(0)pq}, \Pi'_{(0)pq}$ have the form of loops

$'\Phi(mr) =$ 

$'\Psi(mr,np) =$ 

(6.9)

where $((mr) \neq (np))$, corresponding to the following contributions

$$'\Phi(mr) = \frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} G^{\sigma}_{mr,mr}(\mathbf{k}_1,\omega_{n_1})\, t_{\mathbf{q}+\mathbf{k}_1}\Gamma^{\sigma}_{mr}(\mathbf{q}+\mathbf{k}_1,\bar{\omega}_n+\omega_{n_1}), \tag{6.10}$$

$$'\Psi(mr,np) = \frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} \tilde{G}^{\sigma}_{mr,np}(\mathbf{k}_1,\omega_{n_1})\, t_{\mathbf{q}+\mathbf{k}_1}\Gamma^{\sigma}_{mr}(\mathbf{q}+\mathbf{k}_1,\bar{\omega}_n+\omega_{n_1}).$$

Decomposition of the functions G^{σ} and Γ^{σ} in simple fractions and subsequent evaluation of sum over frequency according to (6.5) leads to the expressions like (6.4).

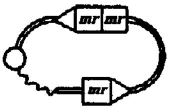
Using

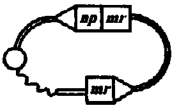
$$\Gamma^{\sigma}_{pq}(\mathbf{k},\omega_n) \approx \frac{1}{i\omega_n - \varepsilon_{pq}(\mathbf{k})}, \tag{6.11}$$

we find in the independent subband approximation

$$\begin{aligned} '\Phi(mr) &= \frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}+\mathbf{q}} \frac{n_+[\varepsilon_{mr}(\mathbf{k})] - n_+[\varepsilon_{mr}(\mathbf{q}+\mathbf{k})]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{q}+\mathbf{k})}, \\ '\Psi(mr,np) &= \frac{1}{N}\sum_{\mathbf{k}} \frac{B_{mr} t_{\mathbf{k}} t_{\mathbf{k}+\mathbf{q}}}{\varepsilon_{mr}(\mathbf{k}) - \varepsilon_{np}(\mathbf{k})} \cdot \frac{n_+[\varepsilon_{mr}(\mathbf{k})] - n_+[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{k}+\mathbf{q})}. \end{aligned} \tag{6.12}$$

Here, in the same way as above we separate only the terms corresponding to the intraband transitions. It is easy to verify that the expressions for loops

$\Phi'(mr) =$ 

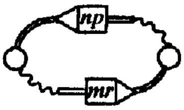
$\Psi'(mr,np) =$ 

(6.13)

entering matrix $\Pi'_{(0)pq}$ are connected with (6.12) by relations

$$\Phi'(mr)\big|_{\bar{\omega}_n} = {}'\Phi(mr)\big|_{-\bar{\omega}_n}; \qquad \Psi'(mr,np)\big|_{\bar{\omega}_n} = {}'\Psi(mr,np)\big|_{-\bar{\omega}_n}. \tag{6.14}$$

Matrix $\Pi_{(0)pq}$. Matrix $\Pi_{(0)pq}$ contains the loops

$\Psi(mr,np) =$ 

(6.15)

as its components. The corresponding expression is

$$\Psi(mr,np) = \frac{1}{\beta}\sum_{n_1}\frac{1}{N}\sum_{\mathbf{k}_1} t_{\mathbf{k}_1} t_{\mathbf{q}+\mathbf{k}_1}\Gamma^{\sigma}_{mr}(\mathbf{k}_1,\omega_{n_1})\Gamma^{\sigma}_{np}(\mathbf{q}+\mathbf{k}_1,\bar{\omega}_n+\omega_{n_1}). \tag{6.16}$$

In the approximation considered here:

$$\Psi(mr,np)=\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}}t_{\mathbf{k}+\mathbf{q}}\frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right]-n_+\left[\varepsilon_{np}(\mathbf{k}+\mathbf{q})\right]}{i\tilde{\omega}_n+\varepsilon_{mr}(\mathbf{k})-\varepsilon_{np}(\mathbf{k}+\mathbf{q})}. \qquad (6.17)$$

This function satisfies the condition

$$\Psi(mr,np)\big|_{\tilde{\omega}_n}=\Psi(np,mr)\big|_{-\tilde{\omega}_n}. \qquad (6.18)$$

The contributions corresponding to loops (6.1) possess the similar symmetry properties

$$\Phi''(mr)\big|_{\tilde{\omega}_n}=\Phi''(mr)\big|_{-\tilde{\omega}_n}; \qquad \Psi''(mr,np)\big|_{\tilde{\omega}_n}=\Psi''(np,mr)\big|_{-\tilde{\omega}_n}. \qquad (6.19)$$

It should be mentioned that all elements of matrices $\left\{\Pi_{(0)}\right\}$ $\left(\Pi''_{(0)}, {}'\Pi_{(0)}, \Pi'_{(0)}, \Pi_{(0)}\right)$ are the even functions of wave–vector $\mathbf{q}$ (if the condition $t_{\mathbf{k}}=t_{-\mathbf{k}}$ is satisfied).

Now let us pass to the analysis of the structure of matrices $\left\{\Pi_{(0)}\right\}$ corresponding to zero–order loops. The selection rules defined by conditions of (5.3) type can be applied in this case. One should also take into account that with the adopted operator priority rules the pairing procedure leading to closed loops of the Fermi–type g–functions adds extra (-1) factor. We can see that, for example, the loop $\Phi''(mr)$ contributes only to the elements $\Pi''_{(0)mm}$, $\Pi''_{(0)rr}$, $\Pi''_{(0)mr}$ and $\Pi''_{(0)rm}$ of matrix $\Pi''_{(0)}$. The contribution to the first two elements enters with minus sign and to the last ones with plus sign. The similar analysis can be performed for all other types of loops. The obtained results are in the table:

$\Phi''(mr)$	mm $-$	rr $-$	mr $+$	rm $+$
$\Psi''(mr,np)$	mn $-$	rp $-$	mp $+$	rn $+$
$'\Phi(mr)$	mm $+$	rr $-$	mr $+$	rm $-$
$'\Psi(mr,np)$	mn $+$	rp $-$	mp $+$	rn $-$
$\Phi'(mr)$	mm $+$	rr $-$	mr $-$	rm $+$
$\Psi'(mr,np)$	nm $+$	pr $-$	nr $-$	pm $+$
$\Psi(mr,np)$	nm $-$	pr $-$	nr $-$	pm $-$

(6.20)

It should be mentioned, that the pairs of indices (mr) take values (41), (23), $(\tilde{4}\tilde{1})$, $(\tilde{2}\tilde{3})$ for the spin direction $\sigma=\uparrow$ and values (31), (24), $(\tilde{3}\tilde{1})$, $(\tilde{2}\tilde{4})$ for $\sigma=\downarrow$.

Then, we can construct matrices $\left\{\Pi_{(0)}\right\}$. The resulting form of matrices $\Pi''^{,\uparrow}_{(0)}$ and $\Pi''^{,\downarrow}_{(0)}$ is given in Appendix A. One can learn from this example how the expressions for other matrices can be constructed with the help of (6.20).

Let us now consider the case of the system where electron pair subbands are well separated from the hole ones ($U \gg g \gg t$). Below half filling (when the electron concentration $n \leq 1$), when double occupied states are absent and the chemical potential is within one of hole subbands, this gives the possibility to consider only the boson correlators or Green functions corresponding to the electron transitions within the set of hole subbands $(41), (\tilde{4}\tilde{1}), (31), (\tilde{3}\tilde{1})$. Then the matrices $\{\Pi^{\sigma}_{(0)}\}$ reduce to the (6×6) dimensionality due to removing of $|2\rangle$ and $|\tilde{2}\rangle$ states. They have the following form

$$\Pi''^{\sigma}_{(0)} = \begin{array}{|c|c|}\hline q_{11}\hat{I}''_{\sigma} & q_{12}\hat{I}''_{\sigma} \\ \hline q_{21}\hat{I}''_{\sigma} & q_{22}\hat{I}''_{\sigma} \\ \hline \end{array} \quad ; \quad {}'\Pi^{\sigma}_{(0)} = \begin{array}{|c|c|}\hline r_{11}{}'\hat{I}_{\sigma} & r_{12}{}'\hat{I}_{\sigma} \\ \hline r_{21}{}'\hat{I}_{\sigma} & r_{22}{}'\hat{I}_{\sigma} \\ \hline \end{array}$$

$$\Pi'^{\sigma}_{(0)} = \begin{array}{|c|c|}\hline s_{11}\hat{I}'_{\sigma} & s_{12}\hat{I}'_{\sigma} \\ \hline s_{21}\hat{I}'_{\sigma} & s_{22}\hat{I}'_{\sigma} \\ \hline \end{array} \quad ; \quad \Pi^{\sigma}_{(0)} = \begin{array}{|c|c|}\hline p_{11}\hat{I}_{\sigma} & p_{12}\hat{I}_{\sigma} \\ \hline p_{21}\hat{I}_{\sigma} & p_{22}\hat{I}_{\sigma} \\ \hline \end{array} \tag{6.21}$$

where (3×3) blocks being their constituent parts. They are formed with the help of matrices

$$\hat{I}''_{\uparrow} = \begin{array}{|c|c|c|}\hline -1 & & 1 \\ \hline & & \\ \hline 1 & & -1 \\ \hline \end{array} \quad ; \quad \hat{I}''_{\downarrow} = \begin{array}{|c|c|c|}\hline -1 & 1 & \\ \hline 1 & -1 & \\ \hline & & \\ \hline \end{array}$$

$$\hat{I}'_{\uparrow} = \begin{array}{|c|c|c|}\hline -1 & & 1 \\ \hline & & \\ \hline -1 & & 1 \\ \hline \end{array} \quad ; \quad \hat{I}'_{\downarrow} = \begin{array}{|c|c|c|}\hline -1 & 1 & \\ \hline -1 & 1 & \\ \hline & & \\ \hline \end{array}$$

$${}'\hat{I}_{\uparrow} = \begin{array}{|c|c|c|}\hline -1 & & -1 \\ \hline & & \\ \hline 1 & & 1 \\ \hline \end{array} \quad ; \quad {}'\hat{I}_{\downarrow} = \begin{array}{|c|c|c|}\hline -1 & -1 & \\ \hline 1 & 1 & \\ \hline & & \\ \hline \end{array} \tag{6.22}$$

$$\hat{I}_{\uparrow} = \begin{array}{|c|c|c|}\hline 1 & & 1 \\ \hline & & \\ \hline 1 & & 1 \\ \hline \end{array} \quad ; \quad \hat{I}_{\downarrow} = \begin{array}{|c|c|c|}\hline 1 & 1 & \\ \hline 1 & 1 & \\ \hline & & \\ \hline \end{array}$$

Here, the following notations are used

$$\begin{aligned}
q_{11} &= \Phi''(41) \quad ; \quad q_{21} = \Psi''(\tilde{4}\tilde{1}, 41) \\
q_{22} &= \Phi''(\tilde{4}\tilde{1}) \quad ; \quad q_{12} = \Psi''(41, \tilde{4}\tilde{1}) \\
r_{11} &= {}'\Phi(41) \quad ; \quad r_{21} = {}'\Psi(\tilde{4}\tilde{1}, 41) \\
r_{22} &= {}'\Phi(\tilde{4}\tilde{1}) \quad ; \quad r_{12} = {}'\Psi(41, \tilde{4}\tilde{1}) \\
s_{11} &= \Phi'(41) \quad ; \quad s_{21} = \Psi'(41, \tilde{4}\tilde{1}) \\
s_{22} &= \Phi'(\tilde{4}\tilde{1}) \quad ; \quad s_{12} = \Psi'(\tilde{4}\tilde{1}, 41) \\
p_{11} &= \Psi(41, 41) \quad ; \quad p_{21} = \Psi(41, \tilde{4}\tilde{1}) \\
p_{22} &= \Psi(\tilde{4}\tilde{1}\tilde{4}\tilde{1}) \quad ; \quad p_{12} = \Psi(\tilde{4}\tilde{1}, 41).
\end{aligned} \tag{6.23}$$

It should be mentioned that we consider nonmagnetic (paramagnetic) state when electron spectrum and semi–invariant averages are degenerated with respect to spin directions.

7 Renormalized polarization loop diagrams

Starting from the obtained expressions for matrices $\left\{\Pi_{(0)}\right\}$ of the zero–order approximation we can find solutions of the eqs.(5.6), (5.7) for the total (renormalized) polarization loops. The results obtained can be written in the following form

$$\begin{aligned}
\Pi^{\prime\prime,\sigma\sigma} &= -\begin{pmatrix} x_{31} & x_{32} \\ x_{41} & x_{42} \end{pmatrix} \times \hat{I}''_{\sigma} \quad ; \quad \Pi^{\prime,\sigma\sigma} = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \times \hat{I}'_{\sigma} \\
{}'\Pi^{\sigma\sigma} &= -\begin{pmatrix} x_{33} & x_{34} \\ x_{43} & x_{44} \end{pmatrix} \times {}'\hat{I}_{\sigma} \quad ; \quad \Pi^{\sigma\sigma} = \begin{pmatrix} x_{13} & x_{14} \\ x_{23} & x_{24} \end{pmatrix} \times \hat{I}_{\sigma} \\
\Pi^{\prime\prime,\sigma,-\sigma} &= -\begin{pmatrix} y_{31} & y_{32} \\ y_{41} & y_{42} \end{pmatrix} \times \hat{I}''_{\sigma,-\sigma} \quad ; \quad \Pi^{\prime,\sigma,-\sigma} = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix} \times \hat{I}'_{\sigma,-\sigma} \\
{}'\Pi^{\sigma,-\sigma} &= -\begin{pmatrix} y_{33} & y_{34} \\ y_{43} & y_{44} \end{pmatrix} \times {}'\hat{I}_{\sigma,-\sigma} \quad ; \quad \Pi^{\sigma,-\sigma} = \begin{pmatrix} y_{13} & y_{14} \\ y_{23} & y_{24} \end{pmatrix} \times \hat{I}_{\sigma,-\sigma},
\end{aligned} \tag{7.1}$$

where

$$\begin{aligned}
\hat{I}''_{\downarrow\uparrow} &= \begin{array}{|c|c|c|} \hline -1 & & 1 \\ \hline 1 & & -1 \\ \hline & & \\ \hline \end{array} \quad ; \quad \hat{I}''_{\uparrow\downarrow} = \begin{array}{|c|c|c|} \hline -1 & 1 & \\ \hline & & \\ \hline 1 & -1 & \\ \hline \end{array} \\
\hat{I}'_{\downarrow\uparrow} &= \begin{array}{|c|c|c|} \hline -1 & & 1 \\ \hline -1 & & 1 \\ \hline & & \\ \hline \end{array} \quad ; \quad \hat{I}'_{\uparrow\downarrow} = \begin{array}{|c|c|c|} \hline -1 & 1 & \\ \hline & & \\ \hline -1 & 1 & \\ \hline \end{array} \\
{}'\hat{I}_{\downarrow\uparrow} &= \begin{array}{|c|c|c|} \hline -1 & & -1 \\ \hline 1 & & 1 \\ \hline & & \\ \hline \end{array} \quad ; \quad {}'\hat{I}_{\uparrow\downarrow} = \begin{array}{|c|c|c|} \hline -1 & -1 & \\ \hline & & \\ \hline 1 & 1 & \\ \hline \end{array} \\
\hat{I}_{\downarrow\uparrow} &= \begin{array}{|c|c|c|} \hline 1 & & 1 \\ \hline 1 & & 1 \\ \hline & & \\ \hline \end{array} \quad ; \quad \hat{I}_{\uparrow\downarrow} = \begin{array}{|c|c|c|} \hline 1 & 1 & \\ \hline & & \\ \hline 1 & 1 & \\ \hline \end{array} .
\end{aligned} \tag{7.2}$$

Quantities x_{ik}, y_{ik} are components of matrices $\hat{X},\hat{Y}$ satisfying the set of equations

$$\hat{X} + \hat{M}\hat{Y} = -\hat{M}; \qquad \hat{Y} + \hat{M}\hat{X} = 0. \tag{7.3}$$

Matrix $\hat{M}$ is formed by the components (6.23) corresponding to the zero-order loops

$$\hat{M} = \begin{pmatrix} s_{11} & s_{12} & p_{11} & p_{12} \\ s_{21} & s_{22} & p_{21} & p_{22} \\ q_{11} & q_{12} & r_{11} & r_{12} \\ q_{21} & q_{22} & r_{21} & r_{22} \end{pmatrix}. \tag{7.4}$$

Formally, the solutions of the set of equations (7.3) are the following

$$\hat{X} = \frac{1}{2}\left(\hat{U} + \hat{V}\right); \qquad \hat{Y} = \frac{1}{2}\left(\hat{U} - \hat{V}\right), \tag{7.5}$$

where

$$\hat{U} = -\left(\hat{1} + \hat{M}\right)^{-1}\hat{M}; \qquad \hat{V} = -\left(\hat{1} - \hat{M}\right)^{-1}\hat{M}. \tag{7.6}$$

The full irreducible parts (5.8) summed up over the spin variables are determined with the help of (7.1) and are represented by block matrices

$$\Pi'' = \begin{array}{|c|c|} \hline \Xi''_{31} & \Xi''_{32} \\ \hline \Xi''_{41} & \Xi''_{42} \\ \hline \end{array} \quad ; \quad \Xi''_{ik} = \begin{array}{|c|c|c|} \hline 2u_{ik} & -u_{ik} & -u_{ik} \\ \hline -u_{ik} & x_{ik} & y_{ik} \\ \hline -u_{ik} & y_{ik} & x_{ik} \\ \hline \end{array}$$

$$\Pi' = \begin{array}{|c|c|}\hline \Xi'_{11} & \Xi'_{12} \\ \hline \Xi'_{21} & \Xi'_{22} \\ \hline \end{array} \quad ; \quad \Xi'_{ik} = \begin{array}{|c|c|c|}\hline 2u_{ik} & -u_{ik} & -u_{ik} \\ \hline u_{ik} & -x_{ik} & -y_{ik} \\ \hline u_{ik} & -y_{ik} & -x_{ik} \\ \hline \end{array}$$

$$'\Pi = \begin{array}{|c|c|}\hline '\Xi_{33} & '\Xi_{34} \\ \hline '\Xi_{43} & '\Xi_{44} \\ \hline \end{array} \quad ; \quad '\Xi_{ik} = \begin{array}{|c|c|c|}\hline 2u_{ik} & u_{ik} & u_{ik} \\ \hline -u_{ik} & -x_{ik} & -y_{ik} \\ \hline -u_{ik} & -y_{ik} & -x_{ik} \\ \hline \end{array} \tag{7.7}$$

$$\Pi = \begin{array}{|c|c|}\hline \Xi_{13} & \Xi_{14} \\ \hline \Xi_{23} & \Xi_{24} \\ \hline \end{array} \quad ; \quad \Xi_{ik} = \begin{array}{|c|c|c|}\hline 2u_{ik} & u_{ik} & u_{ik} \\ \hline u_{ik} & x_{ik} & y_{ik} \\ \hline u_{ik} & y_{ik} & x_{ik} \\ \hline \end{array} .$$

8 Pseudospin, electron, and mixed correlators

Formulae obtained in the previous paragraph complete the evaluation procedure for correlators $\tilde{K}^{pq}$. Expressions for them are determined by the relations (4.17) with matrices (7.7). Here, the total semi–invariants $\bar{\bar{b}}_{pq}$ (sums of chains with loop–like insertions Π) are determined by formula (4.16) where the matrix of second-order semi–invariants $\tilde{b}_{pq}$ for the considered case of $U \gg g \gg t$ has the form

$$\tilde{b} = \begin{array}{|c|c|c|c|c|c|}\hline b_{11} & b_{13} & b_{13} & b_{1\tilde{1}} & b_{1\tilde{3}} & b_{1\tilde{3}} \\ \hline b_{13} & b_{33} & b_{34} & b_{3\tilde{1}} & b_{3\tilde{3}} & b_{3\tilde{4}} \\ \hline b_{13} & b_{34} & b_{33} & b_{3\tilde{1}} & b_{3\tilde{4}} & b_{3\tilde{3}} \\ \hline b_{1\tilde{1}} & b_{3\tilde{1}} & b_{3\tilde{1}} & b_{\tilde{1}\tilde{1}} & b_{\tilde{1}\tilde{3}} & b_{\tilde{1}\tilde{3}} \\ \hline b_{1\tilde{3}} & b_{3\tilde{3}} & b_{3\tilde{4}} & b_{\tilde{1}\tilde{3}} & b_{\tilde{3}\tilde{3}} & b_{\tilde{3}\tilde{4}} \\ \hline b_{1\tilde{3}} & b_{3\tilde{4}} & b_{3\tilde{3}} & b_{\tilde{1}\tilde{3}} & b_{\tilde{3}\tilde{4}} & b_{\tilde{3}\tilde{3}} \\ \hline \end{array} . \tag{8.1}$$

Here, we take into account (see, (3.3)) that $b_{pq} = b_{qp}$. Invariance with respect to electron spin reverse is taken into account too. In zero–order approximation

$$b_{pq} = b_p \delta_{pq} - b_p b_q, \tag{8.2}$$

as it follows from the definition (3.3).

Starting from formulae (7.7) and (8.1) we can rewrite components of correlator $\tilde{K}^{pp'}$ in the explicit form using relation (4.17). It must be taken into account that passing to the momentum–frequency representation we have

$$\tilde{b}_{pp'} \Rightarrow \beta\delta\left(\tilde{\omega}_n\right)\tilde{b}_{pp'}. \tag{8.3}$$

The same applies to the components of matrix $\bar{\bar{b}}_{pp'}$ (this matrix, as well as $\tilde{b}_{pp'}$, is symmetric with respect to the indices pp').

Hence, it follows from (4.16) and (4.17) that

$$\tilde{K}^{pp'}\left(\tilde{\omega}_n, \mathbf{q}\right) = \beta \left\{ \bar{\bar{b}}_{pp'}(\mathbf{q}) + \left[{}'\Pi(0,\mathbf{q})\bar{\bar{b}}(\mathbf{q})\right]_{pp'} + \left[\bar{\bar{b}}(\mathbf{q})\Pi'(0,\mathbf{q})\right]_{pp'} + \right.$$

$$\left. \left[{}'\Pi(0,\mathbf{q})\bar{\bar{b}}(\mathbf{q})\Pi'(0,\mathbf{q})\right]_{pp'} \right\} \delta\left(\tilde{\omega}_n\right) + \Pi''_{pp'}\left(\tilde{\omega}_n, \mathbf{q}\right), \tag{8.4}$$

$$\bar{\bar{b}}_{pp'}(\mathbf{q}) = \left[\left(1 - \beta\tilde{b}\Pi(0,\mathbf{q})\right)^{-1} \tilde{b} \right]_{pp'} . \tag{8.5}$$

Structure of this expression shows the existence of contributions from either localized or collectivized states. The first ones are proportional to $\beta\delta\left(\tilde{\omega}_n\right)$ (of the Curie type) and have static nature. The second one exists at $\tilde{\omega}_n \neq 0$ as well. Such feature of the correlators for the system described by the ordinary Hubbard model was pointed out in [18] in connection with calculation of the magnetic susceptibility.

The contribution into the dynamic susceptibility comes only from the last term in (8.4) corresponding to the full polarization loops Π''.

Let us consider now the expressions for correlators K^{SS}, K^{Sn}, K^{nn} which can be evaluated starting from the relation (8.4) using formulas (2.5) and (2.2). After corresponding summations, we obtain

$$\sum_{p}{}^{(n)}\sum_{p'}{}^{(n)}\bar{\bar{b}}_{pp'} = 2\left(\bar{\bar{b}}_{33} + \bar{\bar{b}}_{34}\right) + 4\left(\bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right) + 2\left(\bar{\bar{b}}_{\tilde{3}\tilde{3}} + \bar{\bar{b}}_{\tilde{3}\tilde{4}}\right),$$

$$\sum_{p}{}^{(S)}\sum_{p'}{}^{(n)}\bar{\bar{b}}_{pp'} = \sum_{p}{}^{(n)}\sum_{p'}{}^{(S)}\bar{\bar{b}}_{pp'} = 2\left(b_{1\tilde{4}} - b_{\tilde{1}3}\right),$$

$$\sum_{p}{}^{(S)}\sum_{p'}{}^{(S)}\bar{\bar{b}}_{pp'} = \bar{\bar{b}}_{11} + 4\bar{\bar{b}}_{13} + 2\bar{\bar{b}}_{33} + 2\bar{\bar{b}}_{34}, \tag{8.6}$$

$$\sum_{p}{}^{(n)}\sum_{p'}{}^{(n)}\Pi''_{pp'} = 2\left(u_{31} + u_{32} + u_{41} + u_{42}\right), \tag{8.7}$$

$$\sum_{p}{}^{(S)}\sum_{p'}{}^{(n)}\Pi''_{pp'} = \sum_{p}{}^{(n)}\sum_{p'}{}^{(S)}\Pi''_{pp'} = \sum_{p}{}^{(S)}\sum_{p'}{}^{(S)}\Pi''_{pp'} = 0,$$

$$\begin{aligned}\sum_{p}{}^{(n)}\sum_{p'}{}^{(n)}\left({}'\Pi\bar{\bar{b}}\right)_{pp'} &= \\ &-2\left(u_{33} + u_{43}\right)\left(2\bar{\bar{b}}_{13} + 2\bar{\bar{b}}_{1\tilde{3}} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right) - \\ &2\left(u_{34} + u_{44}\right)\left(2\bar{\bar{b}}_{3\tilde{1}} + 2\bar{\bar{b}}_{\tilde{1}\tilde{3}} + \bar{\bar{b}}_{\tilde{3}\tilde{3}} + \bar{\bar{b}}_{\tilde{3}\tilde{4}} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right),\end{aligned}$$

$$\begin{aligned}\sum_{p}{}^{(n)}\sum_{p'}{}^{(S)}\left({}'\Pi\bar{\bar{b}}\right)_{pp'} &= -2\left(u_{33} + u_{43}\right)\left(\bar{\bar{b}}_{11} + 3\bar{\bar{b}}_{13} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34}\right) - \\ &2\left(u_{34} + u_{44}\right)\left(\bar{\bar{b}}_{1\tilde{1}} + 2\bar{\bar{b}}_{3\tilde{1}} + \bar{\bar{b}}_{1\tilde{3}} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right),\end{aligned} \tag{8.8}$$

$$\sum_{p}{}^{(S)}\sum_{p'}{}^{(n)}\left({}'\Pi\bar{\bar{b}}\right)_{pp'} = \sum_{p}{}^{(S)}\sum_{p'}{}^{(S)}\left({}'\Pi\bar{\bar{b}}\right)_{pp'} = 0,$$

$$\begin{aligned}\sum_{p}{}^{(n)}\sum_{p'}{}^{(n)}\left(\bar{\bar{b}}\Pi'\right)_{pp'} &= \\ &-2\left(u_{11} + u_{12}\right)\left(2\bar{\bar{b}}_{13} + 2\bar{\bar{b}}_{1\tilde{3}} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right) - \\ &2\left(u_{21} + u_{22}\right)\left(2\bar{\bar{b}}_{3\tilde{1}} + 2\bar{\bar{b}}_{\tilde{1}\tilde{3}} + \bar{\bar{b}}_{\tilde{3}\tilde{3}} + \bar{\bar{b}}_{\tilde{3}\tilde{4}} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right),\end{aligned} \tag{8.9}$$

$$\begin{aligned}\sum_{p}{}^{(S)}\sum_{p'}{}^{(n)}\left(\bar{\bar{b}}\Pi'\right)_{pp'} &= -2\left(u_{11} + u_{12}\right)\left(\bar{\bar{b}}_{11} + 3\bar{\bar{b}}_{13} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34}\right) - \\ &2\left(u_{21} + u_{22}\right)\left(\bar{\bar{b}}_{1\tilde{1}} + 2\bar{\bar{b}}_{3\tilde{1}} + \bar{\bar{b}}_{1\tilde{3}} + \bar{\bar{b}}_{3\tilde{3}} + \bar{\bar{b}}_{3\tilde{4}}\right),\end{aligned}$$

$$\sum_{p}{}^{(n)}\sum_{p'}{}^{(S)}\left(\bar{\bar{b}}\Pi'\right)_{pp'} = \sum_{p}{}^{(S)}\sum_{p'}{}^{(S)}\left(\bar{\bar{b}}\Pi'\right)_{pp'} = 0,$$

$$\begin{aligned}
&\sum_{p}{}^{(n)}\sum_{p'}{}^{(n)}\left('\Pi\bar{\bar{b}}\Pi'\right)_{pp'} = \\
&\quad 2\left(u_{33}+u_{43}\right)\left(u_{11}+u_{12}\right)\left(2\bar{\bar{b}}_{11}+4\bar{\bar{b}}_{13}+\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}\right)+ \\
&\quad 2\left[\left(u_{33}+u_{43}\right)\left(u_{21}+u_{22}\right)+\left(u_{34}+u_{44}\right)\left(u_{11}+u_{12}\right)\right]\times \\
&\quad \left(2\bar{\bar{b}}_{1\tilde{1}}+2\bar{\bar{b}}_{3\tilde{1}}+2\bar{\bar{b}}_{1\tilde{3}}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}\right)+ \\
&\quad 2\left(u_{34}+u_{44}\right)\left(u_{21}+u_{22}\right)\left(2\bar{\bar{b}}_{\tilde{1}\tilde{1}}+4\bar{\bar{b}}_{\tilde{1}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{4}}\right),
\end{aligned} \tag{8.10}$$

$$\left[\sum_{p}{}^{(S)}\sum_{p'}{}^{(n)}+\sum_{p}{}^{(n)}\sum_{p'}{}^{(S)}+\sum_{p}{}^{(S)}\sum_{p'}{}^{(S)}\right]\left('\Pi\bar{\bar{b}}\Pi'\right)_{pp'} = 0.$$

Here, we introduce the notation

$$\sum_{p}{}^{(S)} = \frac{1}{2}\left(\sum_{p=1}^{4}-\sum_{p=\tilde{1}}^{\tilde{4}}\right); \qquad \sum_{p}{}^{(n)} = \sum_{p=3,4,\tilde{3},\tilde{4}} . \tag{8.11}$$

Besides, the property

$$\sum_{p}\bar{\bar{b}}_{pp'} = \sum_{p'}\bar{\bar{b}}_{pp'} = 0. \tag{8.12}$$

which follows from the condition $\sum_p X^{pp} = 1$ and the definition of semi–invariant averages is also taken into account.

In the result

$$K^{AA'} = \sum_{p}{}^{(A)}\sum_{p'}{}^{(A')}\bar{K}^{pp'}, \tag{8.13}$$

where $A, A' = S$ or n. In particular,

$$K^{SS}\left(\bar{\omega}_n,\mathbf{q}\right) = \beta\left(\bar{\bar{b}}_{11}+4\bar{\bar{b}}_{13}+2\bar{\bar{b}}_{33}+2\bar{\bar{b}}_{34}\right)\delta\left(\bar{\omega}_n\right), \tag{8.14}$$

$$\begin{aligned}
K^{Sn}\left(\bar{\omega}_n,\mathbf{q}\right) = \beta\Big[&2\left(\bar{\bar{b}}_{13}+\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}+\bar{\bar{b}}_{1\tilde{3}}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}\right)- \\
&2\left(u_{11}+u_{12}\right)\left(\bar{\bar{b}}_{11}+3\bar{\bar{b}}_{13}+\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}\right)- \\
&2\left(u_{21}+u_{22}\right)\left(\bar{\bar{b}}_{1\tilde{1}}+2\bar{\bar{b}}_{3\tilde{1}}+\bar{\bar{b}}_{1\tilde{3}}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}\right)\Big]\delta\left(\bar{\omega}_n\right),
\end{aligned} \tag{8.15}$$

$$\begin{aligned}
K^{nn}\left(\bar{\omega}_n,\mathbf{q}\right) = \beta\Big[&2\left(\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}+\bar{\bar{b}}_{\tilde{3}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{4}}+2\bar{\bar{b}}_{3\tilde{3}}+2\bar{\bar{b}}_{3\tilde{4}}\right)- \\
&2\left(u_{11}+u_{12}+u_{33}+u_{43}\right)\left(2\bar{\bar{b}}_{13}+2\bar{\bar{b}}_{1\tilde{3}}+\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}\right)- \\
&2\left(u_{21}+u_{22}+u_{34}+u_{44}\right)\left(2\bar{\bar{b}}_{3\tilde{1}}+2\bar{\bar{b}}_{\tilde{1}\tilde{3}}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}+\bar{\bar{b}}_{\tilde{3}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{4}}\right)+ \\
&2\left(u_{33}+u_{43}\right)\left(u_{11}+u_{12}\right)\left(2\bar{\bar{b}}_{11}+4\bar{\bar{b}}_{13}+\bar{\bar{b}}_{33}+\bar{\bar{b}}_{34}\right)+ \\
&2\left[\left(u_{33}+u_{43}\right)\left(u_{21}+u_{22}\right)+\left(u_{34}+u_{44}\right)\left(u_{11}+u_{12}\right)\right]\times \\
&\left(2\bar{\bar{b}}_{1\tilde{1}}+2\bar{\bar{b}}_{3\tilde{1}}+2\bar{\bar{b}}_{1\tilde{3}}+\bar{\bar{b}}_{3\tilde{3}}+\bar{\bar{b}}_{3\tilde{4}}\right)+ \\
&2\left(u_{34}+u_{44}\right)\left(u_{21}+u_{22}\right)\left(2\bar{\bar{b}}_{\tilde{1}\tilde{1}}+4\bar{\bar{b}}_{\tilde{1}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{3}}+\bar{\bar{b}}_{\tilde{3}\tilde{4}}\right)\Big]\delta\left(\bar{\omega}_n\right)+ \\
&2\left(u_{31}+u_{32}+u_{41}+u_{42}\right),
\end{aligned} \tag{8.16}$$

$$K^{nS}(\bar{\omega}_n,\mathbf{q}) = K^{Sn}(\bar{\omega}_n,\mathbf{q}). \tag{8.17}$$

Evidently, the correlators containing pseudospin variable S^z differ from zero only in the static limit ($\bar{\omega}_n = 0$). This is due to the fact that the operator S_i^z commutes with the Hamiltonian being the integral of motion in the case of absence of tunneling splitting ($\Omega = 0$). The corresponding two–time temperature Green functions $\langle\langle S^z|S^z\rangle\rangle_\omega$, $\langle\langle S^z|n\rangle\rangle_\omega$ and $\langle\langle n|S^z\rangle\rangle_\omega$ are equal to zero in this case. We have only

$$K^{nn}(\bar{\omega}_n,\mathbf{q})|_{\bar{\omega}_n\neq 0} = 2\left(u_{31}+u_{32}+u_{41}+u_{42}\right) \tag{8.18}$$

for non–zero frequencies.

It is known that the correlation functions $K^{AA'}(\bar{\omega}_n,\mathbf{q})$ characterize the response of the system to external fields and define its susceptibility. Static and dynamic dielectric susceptibilities are expressed in terms of correlators K^{SS}, K^{nn}, K^{Sn} and K^{nS}. The first one describes the pseudospin (ion) contribution to the so-called transverse susceptibility at $\mu = \text{const}$ regime; the second one describes the pure electron contribution (see Appendix B). Pseudospin component of the susceptibility in the case of fixed electron concentration (regime $n = \text{const}$) has the form

$$\tilde{\chi}^{SS} = K^{SS} - \frac{K^{Sn}K^{nS}}{K^{nn}}, \tag{8.19}$$

the other components are equal zero.

Applying (8.14)–(8.17), we can rewrite formula (8.19) in more explicit form. We introduce notations

$$\begin{aligned} v &= 1 + u_{11} + u_{12} = 1 + u_{33} + u_{43}, \\ w &= 1 + u_{21} + u_{22} = 1 + u_{34} + u_{44} \end{aligned} \tag{8.20}$$

(the latter reflects the symmetry of loops at $\bar{\omega}_n = 0$);

$$\begin{aligned}
\psi_{11} &= 2\bar{\bar{b}}_{11} + 4\bar{\bar{b}}_{13} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34} \\
\psi_{22} &= 2\bar{\bar{b}}_{\bar{1}\bar{1}} + 4\bar{\bar{b}}_{\bar{1}\bar{3}} + \bar{\bar{b}}_{\bar{3}\bar{3}} + \bar{\bar{b}}_{\bar{3}\bar{4}} \\
\psi_{12} &= 2\bar{\bar{b}}_{1\bar{1}} + 2\bar{\bar{b}}_{1\bar{3}} + 2\bar{\bar{b}}_{3\bar{1}} + \bar{\bar{b}}_{3\bar{3}} + \bar{\bar{b}}_{3\bar{4}} \\
\varphi_1 &= \bar{\bar{b}}_{11} + 3\bar{\bar{b}}_{13} + \bar{\bar{b}}_{33} + \bar{\bar{b}}_{34} \\
\varphi_2 &= -\bar{\bar{b}}_{\bar{1}\bar{1}} - 3\bar{\bar{b}}_{\bar{1}\bar{3}} - \bar{\bar{b}}_{\bar{3}\bar{3}} - \bar{\bar{b}}_{\bar{3}\bar{4}} \\
\xi_{11} &= \bar{\bar{b}}_{11}\left(\bar{\bar{b}}_{33} + \bar{\bar{b}}_{34}\right) - 2\bar{\bar{b}}_{13}^{2} \\
\xi_{22} &= \bar{\bar{b}}_{\bar{1}\bar{1}}\left(\bar{\bar{b}}_{\bar{3}\bar{3}} + \bar{\bar{b}}_{\bar{3}\bar{4}}\right) - 2\bar{\bar{b}}_{\bar{1}\bar{4}}^{2} \\
\xi_{12} &= -\bar{\bar{b}}_{1\bar{1}}\left(\bar{\bar{b}}_{3\bar{3}} + \bar{\bar{b}}_{3\bar{4}}\right) + 2\bar{\bar{b}}_{3\bar{1}}\bar{\bar{b}}_{1\bar{3}}.
\end{aligned} \tag{8.21}$$

Then

$$\begin{aligned}
K^{nn} &= 2\beta\left[v^2\psi_{11} + w^2\psi_{22} + 2vw\psi_{12}\right]\delta(\bar{\omega}_n) + K^{nn}_{(d)} \\
K^{Sn} &= K^{nS} = -2\beta\left[v\varphi_1 + w\varphi_2\right]\delta(\bar{\omega}_n) \\
K^{SS} &= \chi^{SS}_{(s)}\delta(\bar{\omega}_n)
\end{aligned} \tag{8.22}$$

and

$$\tilde{\chi}^{SS} = \frac{2\beta^2\left[v^2\xi_{11} + w^2\xi_{22} + 2vw\xi_{12}\right] + \chi^{SS}_{(s)}K^{nn}_{(d)}}{2\beta\left[v^2\psi_{11} + w^2\psi_{22} + 2vw\psi_{12}\right] + K^{nn}_{(d)}}\delta\left(\bar{\omega}_n\right). \tag{8.23}$$

Here

$$K^{nn}_{(d)} = 2\left(u_{31} + u_{32} + u_{41} + u_{42}\right) \tag{8.24}$$

is the dynamic part of the susceptibility;

$$\chi^{SS}_{(s)} = \beta\left(\bar{\bar{b}}_{11} + 4\bar{\bar{b}}_{13} + 2\bar{\bar{b}}_{33} + 2\bar{\bar{b}}_{34}\right) \tag{8.25}$$

is the static pseudospin susceptibility for $\mu = \text{const}$.

9 Matrices of the total pair semi–invariants

Formulae obtained in the previous paragraph give general expressions for correlators $K^{AA'}$. It remains only to consider the matrix of total pair semi–invariants $\bar{\bar{b}}_{pq}$. Formally it is settled by formula (4.16) which follows from the Dyson equation (4.14)

$$\bar{\bar{b}} = b + b\Pi\bar{\bar{b}}, \text{ or } \bar{\bar{b}} = b + \bar{\bar{b}}\Pi b. \tag{9.1}$$

Let us write the matrix equation (9.1) for the Fourier components in the explicit form

$$\bar{\bar{b}}_{pp'} = b_{pp'} + \beta\sum_r \bar{\bar{b}}_{pr}(\Pi b)_{rp'}. \tag{9.2}$$

On the basis of (7.7), (8.1) we have

$$\beta\Pi b = \begin{pmatrix} 2\eta & \bar{\beta}+\zeta & \bar{\beta}+\zeta & 2\psi & \mu+\nu & \mu+\nu \\ \eta & \bar{\beta} & \zeta & \psi & \mu & \nu \\ \eta & \zeta & \bar{\beta} & \psi & \nu & \mu \\ 2\bar{\psi} & \bar{\mu}+\bar{\nu} & \bar{\mu}+\bar{\nu} & 2\pi & \delta+\kappa & \delta+\kappa \\ \bar{\psi} & \bar{\mu} & \bar{\nu} & \pi & \delta & \kappa \\ \bar{\psi} & \bar{\nu} & \bar{\mu} & \pi & \kappa & \delta \end{pmatrix}, \tag{9.3}$$

where

$$\begin{aligned} \eta &= \beta\left[u_{13}\left(b_{11} + b_{13}\right) + u_{14}\left(b_{1\tilde{1}} + b_{1\tilde{3}}\right)\right] \\ \bar{\beta} &= \beta\left[u_{13}b_{13} + x_{13}b_{33} + y_{13}b_{34} + u_{14}b_{\tilde{1}3} + x_{14}b_{3\tilde{3}} + y_{14}b_{3\tilde{4}}\right] \\ \psi &= \beta\left[u_{13}\left(b_{1\tilde{1}} + b_{3\tilde{1}}\right) + u_{14}\left(b_{\tilde{1}\tilde{1}} + b_{\tilde{1}\tilde{3}}\right)\right] \\ \mu &= \beta\left[u_{13}b_{1\tilde{3}} + x_{13}b_{3\tilde{3}} + y_{13}b_{3\tilde{4}} + u_{14}b_{\tilde{1}\tilde{3}} + x_{14}b_{\tilde{3}\tilde{3}} + y_{14}b_{\tilde{3}\tilde{4}}\right], \end{aligned} \tag{9.4}$$

$$\begin{aligned} \zeta &= \bar{\beta}(x \to y, y \to x) \quad &;\quad \nu &= \mu(x \to y, y \to x) \\ \bar{\psi} &= \eta\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \quad &;\quad \pi &= \psi\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \\ \bar{\mu} &= \bar{\beta}\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \quad &;\quad \delta &= \mu\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \\ \bar{\nu} &= \zeta\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \quad &;\quad \kappa &= \nu\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right). \end{aligned}$$

Components (9.4) have the following properties

$$\eta+\bar{\beta}+\zeta+\psi+\mu+\nu=0, \quad \bar{\psi}+\bar{\mu}+\bar{v}+\pi+\delta+\kappa=0. \tag{9.5}$$

The solutions of the set of equations (9.2) can be presented as ($p = 1,\ldots,\tilde{4}$)

$$\begin{aligned}
\bar{\bar{b}}_{p1} &= b_{p1}+\frac{\eta}{\mathrm{Det}_+}\,[1]+\frac{\bar{\psi}}{\mathrm{Det}_+}\,[2]\\
\bar{\bar{b}}_{p\tilde{1}} &= b_{p\tilde{1}}+\frac{\psi}{\mathrm{Det}_+}\,[1]+\frac{\pi}{\mathrm{Det}_+}\,[2]\\
\bar{\bar{b}}_{p3}+\bar{\bar{b}}_{p4} &= b_{p3}+b_{p4}+\frac{\bar{\beta}+\zeta}{\mathrm{Det}_+}\,[1]+\frac{\bar{\mu}+\bar{\nu}}{\mathrm{Det}_+}\,[2]\\
\bar{\bar{b}}_{p\tilde{3}}+\bar{\bar{b}}_{p\tilde{4}} &= b_{p\tilde{3}}+b_{p\tilde{4}}+\frac{\mu+\nu}{\mathrm{Det}_+}\,[1]+\frac{\delta+\kappa}{\mathrm{Det}_+}\,[2]\\
\bar{\bar{b}}_{p3}-\bar{\bar{b}}_{p4} &= \frac{1}{\mathrm{Det}_-}\,[3]\,; \qquad \bar{\bar{b}}_{p\tilde{3}}-\bar{\bar{b}}_{p\tilde{4}}=\frac{1}{\mathrm{Det}_-}\,[4]\,,
\end{aligned} \tag{9.6}$$

with

$$\begin{aligned}
&[1]=(2b_{p1}+b_{p3}+b_{p4})\,(1-2\pi-\delta-\kappa)+\left(2b_{p\tilde{1}}+b_{p\tilde{3}}+b_{p\tilde{4}}\right)(2\bar{\psi}+\bar{\mu}+\bar{\nu})\\
&[2]=\left(2b_{p\tilde{1}}+b_{p\tilde{3}}+b_{p\tilde{4}}\right)(1-2\eta-\bar{\beta}-\zeta)+(2b_{p1}+b_{p3}+b_{p4})\,(2\psi+\mu+\nu)\\
&[3]=(b_{p3}-b_{p4})\,(1-\delta+\kappa)+\left(b_{p\tilde{3}}-b_{p\tilde{4}}\right)(\bar{\mu}-\bar{\nu})\\
&[4]=\left(b_{p\tilde{3}}-b_{p\tilde{4}}\right)(1-\bar{\beta}+\zeta)+(b_{p3}-b_{p4})\,(\mu-\nu)
\end{aligned} \tag{9.7}$$

and also

$$\begin{aligned}
\mathrm{Det}_+ &= (1-2\eta-\bar{\beta}-\zeta)\,(1-2\pi-\delta-\kappa)-(2\psi+\mu+\nu)\,(2\bar{\psi}+\bar{\mu}+\bar{\nu})\\
\mathrm{Det}_- &= (1-\bar{\beta}+\zeta)\,(1-\delta+\kappa)-(\mu-\nu)\,(\bar{\mu}-\bar{\nu})\,.
\end{aligned} \tag{9.8}$$

Substitution of the relation (9.6) into (8.14) – (8.17) leads to the final expressions for correlators $K^{AA'}$.

10 Static correlation functions

The calculation of the polarization loops and corresponding correlators $\bar{K}^{pq}$ and $K^{AA'}$ will be performed for three cases which correspond to the different values of asymmetry parameter of local anharmonic well h. As one can see from fig. 1 the band picture which is determined by the poles of single–electron Green functions suffers principle changes at $h = 0$ and $h = g$. When the tunnelling splitting is absent ($\Omega = 0$), the chemical potential is within the lower subband ($\tilde{4}\tilde{1}$) at $h < 0$, in the upper subband (41) at $h > g$ and for values $0 < h < g$ it is located between subbands and is fixed on the line $\lambda_{\tilde{4}} - \lambda_1$ at $\Omega \to 0$ (see [9]). The average number of electrons per site n being in the range [0,1] in this case.

In this section we shall consider only the static limit $\bar{\omega}_n \to 0$ determining the contributions to the correlation functions.

1. $h > g$. For the considered case we have

$$n_+\left[\varepsilon_{\bar{4}\bar{1}}(\mathbf{k})\right] = 1; \quad n_+\left[\varepsilon_{41}(\mathbf{k})\right] = \begin{cases} 1, & \varepsilon_{41}(\mathbf{k}) < \mu \\ 0, & \varepsilon_{41}(\mathbf{k}) > \mu \end{cases} \tag{10.1}$$

at $T = 0$. It follows from (6.7), (6.12) and (6.17) that at sufficiently low temperatures we can put

$$q_{22} = 0; \quad r_{22} = 0; \quad r_{21} = 0; \quad p_{22} = 0; \quad s_{22} = 0; \quad s_{12} = 0. \tag{10.2}$$

In the limit $\bar{\omega}_n \to 0$ we have

$$s_{11} = r_{11}; \quad s_{21} = r_{12}; \quad p_{12} = p_{21}. \tag{10.3}$$

Besides, we can take into account that the quantities $q_{12} = q_{21}$ contain the ratio $t^2/\left(\lambda_{41} - \lambda_{\bar{4}\bar{1}}\right)^2 \simeq W^2/g^2$ as a factor (W is the width of the initial electron band) for which the relation $W^2/g^2 \ll 1$ is satisfied in the case when the considered subbands can be treated as independent ones. This gives the possibility to put $q_{12} = q_{21} = 0$ when we neglect the contributions of the corresponding small order of magnitude solving the set of equations (7.3).

Finally, for the matrix $\hat{M}$ we obtain

$$\hat{M} = \begin{pmatrix} d & 0 & \varphi & \psi \\ \bar{f} & 0 & \psi & 0 \\ a & 0 & d & \bar{f} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{10.4}$$

where

$$a = q_{11}; \quad d = r_{11}; \quad \bar{f} = r_{12}; \quad \varphi = p_{11}; \quad \psi = p_{12}. \tag{10.5}$$

Substituting (10.4) into (7.3), we obtain after the corresponding transformations

$$u_{ik} = \frac{u^+_{1k}}{\det_+}; \quad v_{ik} = \frac{u^-_{1k}}{\det_-}; \tag{10.6}$$

$$\begin{aligned} u^\pm_{11} &= -d(1 \pm d) \pm \varphi a &&;\quad u^\pm_{13} = -\varphi \\ u^\pm_{21} &= -\bar{f}(1 \pm d) \pm \psi a &&;\quad u^\pm_{23} = -\psi(1 \pm d) \pm \bar{f}\varphi \\ u^\pm_{31} &= -a &&;\quad u^\pm_{33} = -d(1 \pm d) \pm \varphi a \\ u^\pm_{14} &= -\psi(1 \pm d) \pm \varphi\bar{f} &&;\quad u^\pm_{34} = -\bar{f}(1 \pm d) \pm \psi a \\ u^\pm_{24} &= \pm 2\bar{f}\psi(1 \pm d) - \varphi^2 a - \bar{f}^2\varphi &&;\quad u^\pm_{4k} = u^\pm_{i2} = 0, \end{aligned} \tag{10.7}$$

where

$$\det_\pm = (1 \pm d)^2 - \varphi a. \tag{10.8}$$

Using the obtained expressions and formula (9.6) we can calculate combinations of components $\bar{\bar{b}}_{pp'}$ entering (8.21) and (8.25). Let us take into account that

$$b_{\bar{1}} = \left\langle X^{\bar{1}\bar{1}} \right\rangle = 0 \tag{10.9}$$

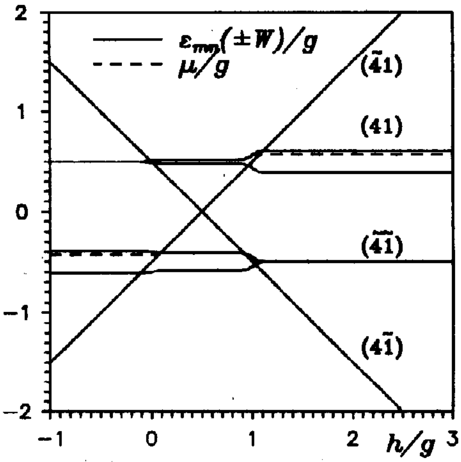


Figure 1: The single–electron bands and chemical potential μ as the functions of the dimensionless coupling strength h/g ($U \to \infty$, $\Omega = 0$, $T/g = 0.03$, $W/g = 0.2$, $n = 0.9$).

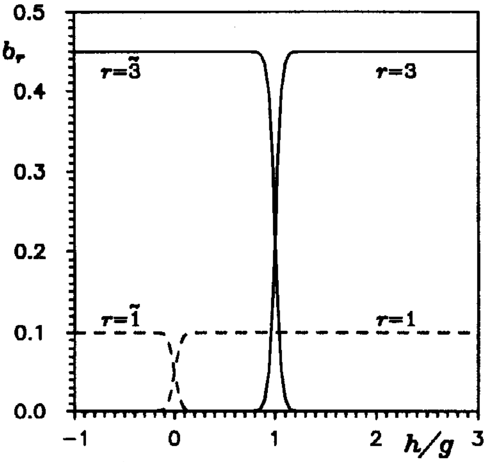


Figure 2: The semi–invariants b_r as the functions of the dimensionless coupling strength h/g ($U \to \infty$, $\Omega = 0$, $T/g = 0.03$, $W/g = 0.2$, $n = 0.9$).

in the considered case (see fig. 2). Expressions for the quantities (9.4) are simplified if we use the functions of zero approximation for $b_{pp'}$. Allowing for (8.2) and (3.3) we get

$$\begin{aligned} \eta &= \beta\left[u_{13}\left(b_{11}+b_{13}\right)+u_{14}b_{1\bar{3}}\right], \\ \bar{\beta}+\zeta &= \beta\left[u_{13}\left(2b_{13}+b_{33}+b_{34}\right)+u_{14}\left(b_{3\tilde{3}}+b_{3\tilde{4}}\right)\right], \\ \mu+\nu &= \beta\left[u_{13}\left(2b_{1\tilde{3}}+b_{3\tilde{3}}+b_{4\tilde{3}}\right)+u_{14}\left(b_{\bar{3}\tilde{3}}+b_{\bar{3}\tilde{4}}\right)\right], \end{aligned} \qquad (10.10)$$

$$\begin{aligned} \bar{\psi} = \eta\left(u_{13}\to u_{23}, u_{14}\to u_{24}\right) \quad &; \quad \bar{\mu}+\bar{\nu} = \left(\bar{\beta}+\zeta\right)\left(u_{13}\to u_{23}, u_{14}\to u_{24}\right) \\ \psi = \pi = 0 \quad &; \quad \delta+\kappa = \left(\mu+\nu\right)\left(u_{13}\to u_{23}, u_{14}\to u_{24}\right). \end{aligned}$$

After the corresponding transformations, this gives the possibility to obtain

$$\begin{aligned} \mathrm{Det}_{+} = 1-\beta(1-n)\left[\frac{n}{2}u_{13}+\left(3u_{13}+u_{24}-4u_{14}\right)b_{\bar{3}}\right]+ \qquad (10.11) \\ 2\beta\left(2u_{14}-u_{13}-u_{24}\right)b_{3}b_{\bar{3}}-\beta^{2}(1-n)\left(u_{14}^{2}-u_{13}u_{24}\right)b_{3}b_{\bar{3}}, \end{aligned}$$

$$\bar{\bar{b}}_{11}+4\bar{\bar{b}}_{13}+2\bar{\bar{b}}_{33}+2\bar{\bar{b}}_{34} = \frac{1}{\mathrm{Det}_{+}}\left[2(1-n)b_{\bar{3}}+4b_{3}b_{\bar{3}}-2(1-n)u_{13}\beta b_{3}b_{\bar{3}}\right]. \qquad (10.12)$$

Using (8.21) and (8.25), we have

$$K^{SS}\left(\bar{\omega}_{n},\mathbf{q}\right) = \frac{\beta}{\mathrm{Det}_{+}}\left[2(1-n)b_{\bar{3}}+4b_{3}b_{\bar{3}}-2(1-n)u_{13}\beta b_{3}b_{\bar{3}}\right]\delta\left(\bar{\omega}_{n}\right), \qquad (10.13)$$

respectively. The correlators K^{nn}, K^{Sn} and K^{nS} can be expressed in the same way with the help of formula (9.6) and (9.4).

2. $h < 0$. The chemical potential is in the lower subband for $T = 0$

$$n_+\left[\varepsilon_{41}(\mathbf{k})\right] = 0; \quad n_+\left[\varepsilon_{\tilde{4}\tilde{1}}(\mathbf{k})\right] = \begin{cases} 1, & \varepsilon_{\tilde{4}\tilde{1}}(\mathbf{k}) < \mu \\ 0, & \varepsilon_{\tilde{4}\tilde{1}}(\mathbf{k}) > \mu \end{cases}. \tag{10.14}$$

In this case we can assume

$$q_{11} = 0; \quad r_{11} = 0; \quad r_{12} = 0; \quad p_{11} = 0; \quad s_{11} = 0; \quad s_{21} = 0 \tag{10.15}$$

and $q_{12} \simeq q_{21} \simeq 0$. Besides,

$$s_{22} = r_{22}; \quad s_{12} = r_{21}; \quad p_{12} = p_{21} \tag{10.16}$$

for $\bar{\omega}_n \to 0$.

Matrix $\hat{M}$ now takes the form

$$\hat{M} = \begin{pmatrix} 0 & f & 0 & \bar{\psi} \\ 0 & \bar{g} & \bar{\psi} & \bar{\varphi} \\ 0 & 0 & 0 & 0 \\ 0 & b & f & \bar{g} \end{pmatrix}, \tag{10.17}$$

where

$$b = q_{22}; \quad \bar{g} = r_{22}; \quad f = r_{21}; \quad \bar{\varphi} = p_{22}; \quad \bar{\psi} = p_{12}. \tag{10.18}$$

Solving the set of equations (7.3) with the use of (10.17), we obtain

$$u_{ik} = \frac{u^{+}_{1k}}{\det'_{+}}; \quad v_{ik} = \frac{u^{-}_{1k}}{\det'_{-}}; \tag{10.19}$$

$$\begin{aligned} u^{\pm}_{22} &= -\bar{g}(1 \pm \bar{g}) \pm \bar{\varphi}b \quad ; \quad u^{\pm}_{24} = -\bar{\varphi} \\ u^{\pm}_{12} &= -f(1 \pm \bar{g}) \pm \bar{\psi}b \quad ; \quad u^{\pm}_{14} = -\bar{\psi}(1 \pm \bar{g}) \pm f\bar{\varphi} \\ u^{\pm}_{42} &= -b \quad ; \quad u^{\pm}_{44} = -\bar{g}(1 \pm \bar{g}) \pm \bar{\varphi}b \\ u^{\pm}_{23} &= -\bar{\psi}(1 \pm \bar{g}) \pm \bar{\varphi}f \quad ; \quad u^{\pm}_{43} = -f(1 \pm \bar{g}) \pm \bar{\psi}b \\ u^{\pm}_{13} &= \pm 2f\bar{\psi}(1 \pm \bar{g}) - \bar{\varphi}^2 b - f^2\bar{\varphi} \quad ; \quad u^{\pm}_{3k} = u^{\pm}_{i1} = 0. \end{aligned} \tag{10.20}$$

Here

$$\det'_{\pm} = (1 \pm \bar{g})^2 - \bar{\varphi}b. \tag{10.21}$$

For $h < 0$ and $T \to 0$ we have $b_3 = b_4 = \langle X^{33} \rangle = \langle X^{44} \rangle$. We shall write the expressions for quantities (9.4) taking into account this fact and evaluating semi-invariants $b_{pp'}$ in zeroth approximation in the same way as in paragraph 10.1

$$\begin{aligned} \eta &= \beta\left[u_{13}b_{11} + u_{14}\left(b_{1\tilde{1}} + b_{1\tilde{3}}\right)\right], \\ \psi &= \beta\left[u_{13}b_{1\tilde{1}} + u_{14}\left(b_{\tilde{1}\tilde{1}} + b_{\tilde{1}\tilde{3}}\right)\right], \\ \mu + \nu &= \beta\left[2u_{13}b_{1\tilde{3}} + u_{14}\left(2b_{\tilde{1}\tilde{3}} + b_{\tilde{3}\tilde{3}} + b_{\tilde{3}\tilde{4}}\right)\right], \end{aligned} \tag{10.22}$$

$$\begin{aligned} \bar{\psi} = \eta\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \quad &; \quad \pi = \psi\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right) \\ \bar{\beta} + \zeta = \bar{\mu} + \bar{\nu} = 0 \quad &; \quad \delta + \kappa = (\mu + \nu)\left(u_{13} \to u_{23}, u_{14} \to u_{24}\right). \end{aligned}$$

In particular after substitution of (10.22) into (9.6)–(9.8) we obtain

$$\mathrm{Det}_+ = 1 - \beta n \left[\frac{1-n}{2} u_{24} + 2\left(u_{13} - u_{14}\right) b_1\right] + \qquad (10.23)$$

$$2\beta\left(2u_{14} - u_{13} - u_{24}\right) b_1 b_{\bar{1}} - \beta^2 n \left(u_{14}^2 - u_{13}u_{24}\right) b_1 b_{\bar{1}},$$

$$\bar{\bar{b}}_{11} + 4\bar{\bar{b}}_{13} + 2\bar{\bar{b}}_{33} + 2\bar{\bar{b}}_{34} = \bar{\bar{b}}_{11} = \frac{1}{\mathrm{Det}_+}\left[n b_1 + b_1 b_{\bar{1}} - \frac{n}{2} u_{24}\beta b_1 b_{\bar{1}}\right]. \quad (10.24)$$

This gives the possibility to write

$$K^{SS}\left(\bar{\omega}_n, \mathbf{q}\right) = \frac{\beta}{\mathrm{Det}_+}\left[n b_1 + b_1 b_{\bar{1}} - \frac{n}{2} u_{24}\beta b_1 b_{\bar{1}}\right] \delta\left(\bar{\omega}_n\right). \qquad (10.25)$$

The expressions for other correlators $K^{AA'}$ are obtained in the same way.

3. $0 < h < g$. In this case the chemical potential is located between subbands $(\tilde{4}\bar{1})$ and (41). For $T \to \infty$ we have

$$n_+\left[\varepsilon_{41}(\mathbf{k})\right] = 0; \quad n_+\left[\varepsilon_{\tilde{4}\bar{1}}(\mathbf{k})\right] = 1 \qquad (10.26)$$

for all values of $\mathbf{k}$.

If we restrict ourselves to the contributions up to the first order in powers of W/g we can keep in matrix $\hat{M}$ only components $p_{12} = p_{21}$

$$\hat{M} = \begin{pmatrix} 0 & 0 & 0 & \psi' \\ 0 & 0 & \psi' & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad (10.27)$$

where $\psi' = p_{12}$. Among the quantities $u_{ik}^{\pm}$, only

$$u_{23}^{\pm} = u_{14}^{\pm} = \psi' \qquad (10.28)$$

are different from zero, as it follows from (7.3). This leads to the simpler expressions for quantities (9.4).

Starting from formulas (9.6)–(9.8), we can obtain

$$\mathrm{Det}_+ = 1 + 4u_{14}\beta\left(b_1 + b_3\right)\left(b_{\bar{1}} + b_{\bar{3}}\right) - u_{14}^2\beta^2 b_1 b_{\bar{3}}\left(b_3 + 2b_{\bar{1}}\right), \qquad (10.29)$$

Expression (10.29) is written in the linear approximation with respect to the averages $b_{\bar{1}}$, b_3, for which the relations $b_{\bar{1}} \ll 1$, $b_3 \ll 1$ are satisfied if the values of parameter h are in the interval $[0, g]$.

11 Static susceptibilities χ^{SS}, χ^{nn} and χ^{nS}

The expressions obtained in the previous section become more simple when we use the results of evaluation of quantities (10.7), (10.20) and (10.28) which are the combinations of the matrix elements $\hat{M}$. The calculation procedure is described in the Appendix C. This gives the possibility to write in the explicit form the pseudospin, electron and mixed components of the static susceptibility which for the μ = const regime are determined by the corresponding correlators

$$\chi^{SS} = K^{SS}, \quad \chi^{nn} = K^{nn}, \quad \chi^{nS} = \chi^{Sn} = K^{nS} \tag{11.1}$$

and by

$$\tilde{\chi}^{SS} = K^{SS} - \frac{K^{Sn}K^{nS}}{K^{nn}}, \quad \tilde{\chi}^{Sn} = \tilde{\chi}^{nn} = 0 \tag{11.2}$$

for the regime n = const.

The "transverse" dielectric susceptibility (corresponding to the components ε_{zz} in the normal direction to the layers of YBaCuO structures) is given by the formula

$$\chi_{\perp} = \chi^{PP} = d_S^2\chi^{SS} + d_e^2\chi^{nn} + 2d_e d_S\chi^{Sn}, \tag{11.3}$$

which follows from the definition of the dipole momentum operator of the cell [9]

$$P_i = d_S S_i^z + d_e n_i. \tag{11.4}$$

In the same way as above, let us consider separately the cases $h > g$, $h < 0$ and $0 < h < g$.

1. $h > g$. It follows from eqs. (10.7) and (C.6), that

$$\frac{u_{23}}{u_{13}} = \frac{u_{14}}{u_{13}} \simeq \frac{W}{g}; \quad \frac{u_{21}}{u_{11}} \simeq \frac{W}{g}; \quad \frac{u_{24}}{u_{13}} \simeq \frac{W^2}{g^2}. \tag{11.5}$$

The main contribution into total semi-invariants $\bar{\bar{b}}_{pq}$ (eq. (10.12)) and correlators (8.22) at $W/g \ll 1$ is connected with the quantities u_{13} and u_{11}. So we can put

$$\begin{aligned} \eta &= \beta u_{13}(b_{11} + b_{13}), \\ \bar{\beta} + \zeta &= \beta u_{13}(2b_{13} + b_{33} + b_{34}), \\ \mu + \nu &= \beta u_{13}(2b_{1\bar{3}} + b_{3\bar{3}} + b_{4\bar{3}}), \\ \bar{\psi} = \bar{\mu} + \bar{\nu} &= \delta + \kappa = 0; \quad \psi = \pi = 0, \end{aligned} \tag{11.6}$$

$$v = 1 + u_{11}; \quad w = 1. \tag{11.7}$$

This results in

$$\mathrm{Det}_+ = 1 - u_{13}\beta\left[(1-n)\left(\frac{n}{2} + 3b_{\bar{3}}\right) - v_0\right], \tag{11.8}$$

$$\begin{aligned} \psi_{11} &= \frac{1}{\mathrm{Det}_+}\left[(1-n)\left(\frac{n}{2} + 3b_{\bar{3}}\right) - v_0\right], \\ \psi_{22} &= \frac{1}{\mathrm{Det}_+}\left[(1-n)b_{\bar{3}} - v_0 + \frac{1}{2}u_{13}\beta v_0(1-n)\right], \\ \psi_{12} &= \frac{1}{\mathrm{Det}_+}\left[-2(1-n)b_{\bar{3}} + v_0\right], \end{aligned} \tag{11.9}$$

$$\varphi_1 = 2(1-n)b_{\bar{3}} - v_0 \quad ; \quad \varphi_2 = -\psi_{22}$$

$$\xi_{11} = \frac{1}{\mathrm{Det}_+}v_0(n-1) \quad ; \quad \xi_{22} = \xi_{12} = 0.$$

Here $v_0 = -2b_3b_{\bar{3}}$ and it is taken into consideration that $b_{\bar{1}} \simeq 0$ in the region $h > 0$.

The pseudospin component of susceptibility in this case is equal to

$$\chi^{SS} = \chi^{SS}_{(s)}\delta\left(\bar{\omega}_n\right) = \frac{\beta}{\mathrm{Det}_+}\left[2(1-n)b_{\bar{3}} - 2v_0 + u_{13}\beta v_0(1-n)\right]\delta\left(\bar{\omega}_n\right) \tag{11.10}$$

for $\mu = \text{const}$,

$$\begin{aligned} \tilde{\chi}^{SS} \;=\; & \delta\left(\bar{\omega}_n\right)\Big\{-2\beta^2(1+u_{11})^2v_0(1-n)+ \\ & \beta K^{nn}_{(d)}\left[2(1-n)b_{\bar{3}} - 2v_0 + u_{13}\beta v_0(1-n)\right]\Big\} \times \\ & \Big\{\beta^2u_{13}v_0(1-n) + \beta\left[n(1-n) + 4u_{11}(1-n)\left(\frac{n}{2} + b_{\bar{3}}\right)\right] + \\ & \beta\left(2u_{11}^2 - K^{nn}_{(d)}u_{13}\right)\left[(1-n)\frac{n}{2} + 3(1-n)b_{\bar{3}} - v_0\right] + K^{nn}_{(d)}\Big\}^{-1} \end{aligned} \tag{11.11}$$

for $n = \text{const}$. Correspondingly, we obtain for electron and mixed components

$$\begin{aligned} K^{nn} \;=\; & K^{nn}_{(d)} + \frac{2\beta}{\mathrm{Det}_+}\left[(1-n)\frac{n}{2}\left(1+u_{11}\right)^2 - v_0u_{11}^2 + \right. \\ & \left.(1-n)b_{\bar{1}}\left(2u_{11} + 3u_{11}^2\right) + \frac{1}{2}\beta u_{13}v_0(1-n)\right]\delta\left(\bar{\omega}_n\right), \\ K^{Sn} = K^{nS} \;=\; & \frac{2\beta}{\mathrm{Det}_+}\left[(1-n)b_{\bar{3}}\left(2u_{11} - 1\right) + \right. \\ & \left. u_{11}v_0 + \frac{1}{2}u_{13}\beta v_0(1-n)\right]\delta\left(\bar{\omega}_n\right). \end{aligned} \tag{11.12}$$

2. $h < 0$. In this case the following relations take place

$$\frac{u_{14}}{u_{24}} = \frac{u_{23}}{u_{24}} \simeq \frac{W}{g}; \quad \frac{u_{12}}{u_{22}} \simeq \frac{W}{g}; \quad \frac{u_{13}}{u_{24}} \simeq \frac{W^2}{g^2}. \tag{11.13}$$

If we limit ourselves to the zero–order terms in W/g we find

$$\begin{aligned} \pi = \beta u_{24}\left(b_{\bar{1}\bar{1}} + b_{\bar{1}\bar{3}}\right), \quad \bar{\psi} = \beta u_{24}\left(b_{1\bar{1}} + b_{1\bar{3}}\right), \\ \delta + \kappa = \beta u_{24}\left(2b_{\bar{1}\bar{3}} + b_{\bar{3}\bar{3}} + b_{\bar{3}\bar{4}}\right), \\ \eta = \bar{\beta} + \zeta = \mu = \nu = \psi = \bar{\mu} + \bar{\nu} = 0, \\ v = 1; \quad w = 1 + u_{22}. \end{aligned} \tag{11.14}$$

Using these expressions, let us write in the explicit form the formulae (9.6)–(9.8) and (9.4). Then

$$\mathrm{Det}_+ = 1 - u_{24}\beta\left[(1-n)\frac{n}{2} + 2b_1b_{\bar{1}}\right],$$

$$\begin{aligned}
\psi_{11} &= \frac{2}{\mathrm{Det}_+}\left[b_1\left(n+b_{\bar 1}\right)-u_{24}\beta\frac{n}{2}b_1b_{\bar 1}\right], \\
\psi_{22} &= \frac{1}{\mathrm{Det}_+}\left[(1-n)\frac{n}{2}+2b_1b_{\bar 1}\right], \\
\psi_{12} &= -\frac{1}{\mathrm{Det}_+}b_1\left(n+2b_{\bar 1}\right), \qquad (11.15)\\
\varphi_1 &= \frac{1}{2}\psi_{11} \quad ; \quad \varphi_2=\frac{1}{2}\psi_{12} \\
\xi_{11} &= \xi_{12}=0 \quad ; \quad \xi_{22}=\frac{1}{\mathrm{Det}_+}b_1b_{\bar 1}\frac{n}{2}
\end{aligned}$$

($b_3 = b_4 \simeq 0$ for $h < 0$).

On the basis of (8.21) and (8.23) we find for the pseudospin component of susceptibility

$$\chi^{SS} = \chi^{SS}_{(s)}\delta\left(\bar\omega_n\right) = \frac{\beta}{\mathrm{Det}_+}\left[b_1\left(n+b_{\bar 1}\right)-u_{24}\beta\frac{n}{2}b_1b_{\bar 1}\right]\delta\left(\bar\omega_n\right) \qquad (11.16)$$

for $\mu = \text{const}$;

$$\begin{aligned}
\tilde\chi^{SS} = {} & \left\{2\beta^2(1+u_{22})^2b_1b_{\bar 1}\frac{n}{2}+\right. \\
& \left.\beta K^{nn}_{(d)}\left[b_1\left(n+b_{\bar 1}\right)-u_{24}\beta\frac{n}{2}b_1b_{\bar 1}\right]\right\}\times \qquad (11.17)\\
& \left\{2\beta\left[(1+u_{22})^2\frac{n}{2}(1-n)+2u_{22}^2b_1b_{\bar 1}-2u_{22}b_1n-u_{24}\beta nb_1b_{\bar 1}\right]-\right. \\
& \left.\beta u_{24}\left[\frac{n}{2}(1-n)+2b_1b_{\bar 1}\right]K^{nn}_{(d)}+K^{nn}_{(d)}\right\}^{-1}\delta\left(\bar\omega_n\right)
\end{aligned}$$

for $n = \text{const}$. Then the electron and mixed components have the following form

$$\begin{aligned}
K^{nn} = {} & K^{nn}_{(d)}+\frac{2\beta}{\mathrm{Det}_+}\left[(1-n)\frac{n}{2}\left(1+u_{22}\right)^2+2u_{22}^2b_1b_{\bar 1}-\right. \\
& \left.2u_{22}b_1n-u_{24}\beta nb_1b_{\bar 1}\right]\delta\left(\bar\omega_n\right), \qquad (11.18)\\
K^{Sn} = K^{nS} = {} & -\frac{\beta}{\mathrm{Det}_+}\left[b_1n\left(1-u_{22}\right)-2u_{22}b_1b_{\bar 1}-u_{24}\beta nb_1b_{\bar 1}\right]\delta\left(\bar\omega_n\right).
\end{aligned}$$

12 Numerical calculations and discussion of the results

Starting from the obtained above formulae for susceptibility, we can investigate its behaviour with the change of the thermodynamic parameters (e.g., temperature, electron concentration) and constants of Hamiltonian (h, Ω or g) The corresponding calculations are performed numerically. We shall use the following dimensionless quantities

$$\frac{h}{g},\quad \frac{\Omega}{g},\quad \frac{W}{g},\quad \frac{kT}{g}=\frac{1}{\beta g}, \qquad (12.1)$$

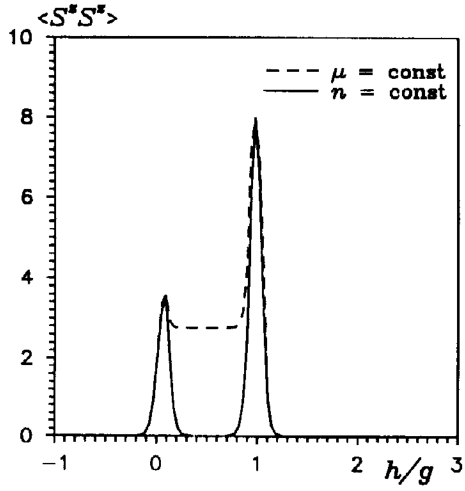


Figure 3: The pseudospin susceptibility $\langle SS \rangle$ as a function of the dimensionless coupling strength h/g ($\Omega = 0$, $T/g = 0.03$, $W/g = 0.2$, $n = 0.9$).

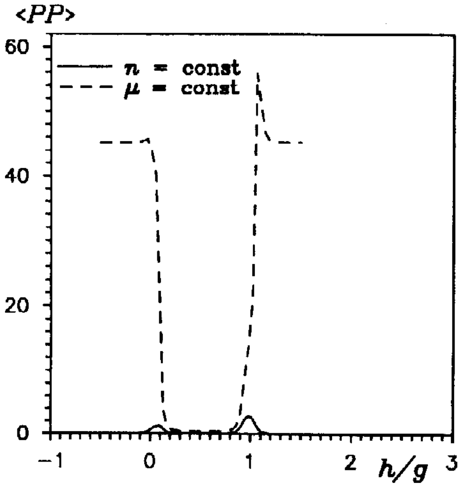


Figure 4: The total susceptibility $\langle PP \rangle$ as a function of the dimensionless coupling strength h/g ($U \to \infty$, $\Omega = 0$, $T/g = 0.03$, $W/g = 0.2$, $n = 0.9$, $d_S/d_e = 0.6$).

where W is the half-width of the initial electron band (at the absence of the correlation and interactions), and

$$\langle SS \rangle = K^{SS} g; \quad \langle PP \rangle = K^{PP} \frac{g}{d_e^2}; \quad \chi = \chi^{PP} \left[\frac{d_e^2}{v_c g} \right]^{-1}. \tag{12.2}$$

We shall start, predominantly in choosing the possible numerical values of parameters, from the data presented in [6,7,20], where the values $g = 10 \div 20$, $\Omega = 0 \div 5$, $W = 0 \div 2$ [6], $g = 1 \div 10$, $\Omega = 1 \div 10$, $W = 1$ [7] and $g = 0.3 \div 0.5$, $\Omega = 0.1$, $W = 1$ [20] were used. This gives $\Omega/g = 0 \div 10$, $W/g = 0 \div 1$. We shall limit ourselves to the case $W/g \ll 1$ in accordance with the independent subband approximation used in this work. We also put $\Omega = 0$. The values of the asymmetry parameter h and temperature kT will be changed in the wide range ($-1 \leq h/g \leq 3$; $0 \leq kT/g \leq 1$). Also, the different possible values of electron concentration n will be considered ($0 \leq n \leq 1$).

The results of the numerical calculations are based on the formulae obtained in the previous sections and are shown in fig. 3–8.

We shall start the analysis from the consideration of the dependencies of the susceptibility vs symmetry of the anharmonic potential (fig. 3 and 4). One can see, that the characteristic feature of the function $\langle SS \rangle_n$ (at $n = \text{const}$) is the existence of two sharp maxima localized near values $h = 0$ and $h = g$. The width of these peaks increases with the increase of T (on the other hand, they tend to δ–function form with decrease of temperature and $W \to 0$). The similar two peak structure of the function $\langle SS \rangle_n$ was revealed in [9] for the $\Omega \neq 0$ case where for the determination of susceptibility the relations

$$\chi_\perp = \begin{cases} \frac{2}{v_c} \left[d_S \left(\frac{\partial \langle S_i^z \rangle}{\partial E_\perp} \right)_\mu + d_e \left(\frac{\partial \langle n_i \rangle}{\partial E_\perp} \right)_\mu \right] & , \mu = \text{const} \\ \frac{2}{v_c} d_S \left(\frac{\partial \langle S_i^z \rangle}{\partial E_\perp} \right)_n & , n = \text{const} \end{cases} \tag{12.3}$$

were used, and the evaluation of derivatives $\frac{\partial\langle X^{pp}\rangle}{\partial E_\perp}$ was performed in Hubbard–I approximation (the broadening of the peak exists in this case even at $T = 0$ and is caused by the tunnelling). The presence of two sharp maxima of function $\langle SS\rangle_n$ in the regions $h \simeq 0$ and $h \simeq g$ testifies the "softening" of the initial crystal structure with respect to the anharmonic degrees of freedom. One can verify that this effect is caused by the cancellation of the fields acting on the pseudospins: the asymmetry field ($\simeq h$) and the field from the electron subsystem which is determined by the occupation of electron states ($\simeq n_r g$; $n_r = 0$ or 1 for $U \to \infty$). If one varies the electron concentration in the range [0,1], then the heights of the peaks redistribute (see fig. 3) and at $n \to 1$ there remains only one peak at $h = g$ while at $n \to 0$ only the second one is present. It should be mentioned that at finite value of correlation energy U and $1 < n < 2$ there appears also the peak at $h = 2g$ with the corresponding value $n_r = 2$.

The behaviour of the susceptibility $\langle SS\rangle_\mu$ (at $\mu = \text{const}$) vs h is somewhat different in comparison with the $\langle SS\rangle_n$ one. Function $\langle SS\rangle_\mu$ achieves a constant value in the region between maxima ($0 < h < g$) and increases with the decrease of temperature (tending to infinity at $T \to 0$). Out of this interval $\langle SS\rangle_\mu$ coinsides in general with $\langle SS\rangle_n$.

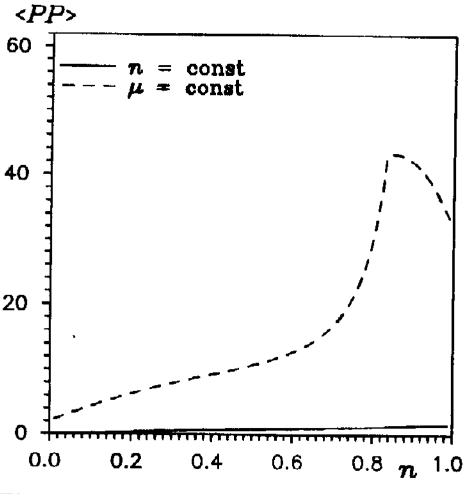


Figure 5: Dependence of total susceptibility $\langle PP\rangle$ on electron concentration n ($U \to \infty$, $h/g = 1.05$, $\Omega = 0$, $W/g = 0.2$, $T/g = 0.03$, $d_S/d_e = 0.6$).

The dependencies of total susceptibility $\langle PP\rangle$ vs h in the regimes $n = \text{const}$ and $\mu = \text{const}$ are presented in fig. 4. The significant increase of the function $\langle PP\rangle_\mu$ at values $h \simeq 0$ and $h \simeq g$ is caused by entering of chemical potential into allowed energy bands and, as the result, by the appearance of the electron component of the susceptibility which is much greater than the pseudospin one (such effect was marked in [9])[1]. In our calculations, the chemical potential was supposed to be given but the appropriate value was chosen to obtain the certain value of electron concentration.

The behaviour of total susceptibility $\langle PP\rangle$ with the change of electron concentration is shown in fig. 5. The case, when h is in the region of right maximum of the function $\langle SS\rangle_n$, was considered. Here, $\langle PP\rangle_\mu / \langle PP\rangle_n \gg 1$ due to the electron component of susceptibility. This ratio achieves its maximum at $n \simeq 0.85$ and rapidly decreases with the decrease of n.

The dependencies of pseudospin and total susceptibilities vs temperature are shown in fig. 6a,b. The difference between the behaviour of function $\langle SS\rangle$ in the regimes $n = \text{const}$ and $\mu = \text{const}$ is not considerable. For $h > g$ (as well as for $h < 0$) the curve $\langle SS\rangle(T)$ has a maximum rapidly decreasing to zero when $T \to 0$ and smoothly decreasing (like Cuerie–Weiss law) at

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[1] For YBaCuO–type structures $d_S = Z(O_A)\delta$, where $\delta \simeq 0.13$ Å is the characteristic size of the anharmonic well (the distance between minima); $d_e \approx eD$, D is the distance between the CuO plain and the plain of Cu–O chains; $d_S \ll d_e$.

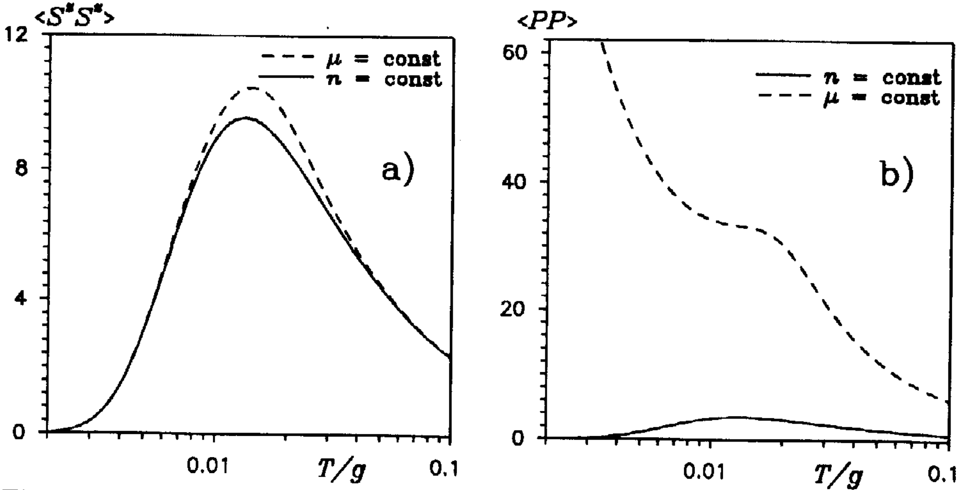

Figure 6: The temperature dependence of $\langle SS\rangle$ (a) and $\langle PP\rangle$ (b) ($U \to \infty$, $h/g = 1.05$, $\Omega = 0$, $W/g = 0.2$, $n = 0.7$, $d_S/d_e = 0.6$).

high temperatures. The total susceptibility $\langle PP\rangle_\mu$ achieves much greater values with strong increase at $T \to 0$.

The peculiarities of the temperature dependencies of functions $\langle SS\rangle_n$ and $\langle SS\rangle_\mu$ (fig. 7) (appearing in the certain range of parameter values) are the essential feature of the model. These peculiarities have the character of divergencies. At $T < T^*$ (where T^* is the temperature at which the peculiarity takes place) susceptibility $\langle SS\rangle$ is negative in the certain temperature range. The existence of such peculiarities can be treated as the manifestation of the dielectric type instabilities appearing in the pseudospin subsystem (i.e. anharmonic oscillators) under the influence of the effective interactions. The denominator in the expression for susceptibility χ^{SS} (eq. (8.5)) becomes zero at temperature T^*. This denominator is connected with the factor $\left(1 - \hat{b}\hat{\Pi}\right)^{-1}$, which appears as the result of the summation of polarization loop series. The total loop $\Pi_{rs}^{(ij)}$ describes the effective interaction between the states $|r\rangle$ and $|s\rangle$ of the cells i and j via conducting electrons.

The dependence of the instability temperature T^* on the electron concentration is shown in fig. 8 for two different values of the electron transfer integral (i.e. initial width of the electron band W). The case $h \geq g$ is taken. It is clear that the effect is caused by the band motion of electrons; T^* decreases with the decrease of W. The graphs presented in fig. 8 can be treated as the phase diagrams with the curves separating regions where the initial state of the system is stable. The problem which state takes place at $T < T^*$ and is there the possibility for the phase transition (e.g. of ferro– or antiferroelectric type) needs additional investigations.

It should be mentioned, that the obtained considerable increase (for the certain region of values of temperature and parameters) of the contributions into transverse dielectric susceptibility from pseudospin and subsystem of electron can be relevant in the problem of interpretation of the onset of superconducting state.[1] As far as the effective interelectron coupling constant λ is proportional to the contribution of the correspondent lattice mode into dielectric susceptibility ($\lambda \simeq N(0)\langle V^2\rangle\chi_S(0)$), the increase of $\chi_S(0)$ and

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[1] It was shown in Refs. [12,13] that high values of dielectric susceptibility occur in YBaCuO compounds.

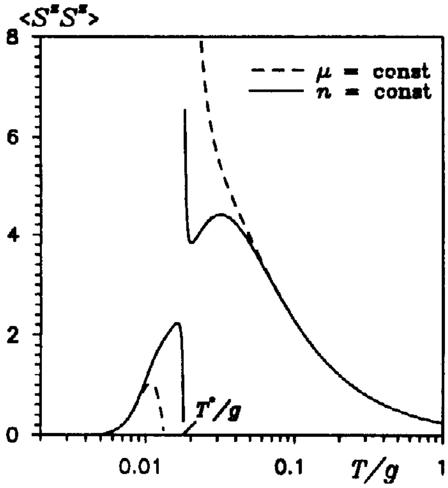

Figure 7: The temperature dependence of $\langle SS\rangle_n$ and $\langle SS\rangle_\mu$ ($U \to \infty$, $h/g = 1.05$, $\Omega = 0$, $W/g = 0.2$, $n = 0.95$).

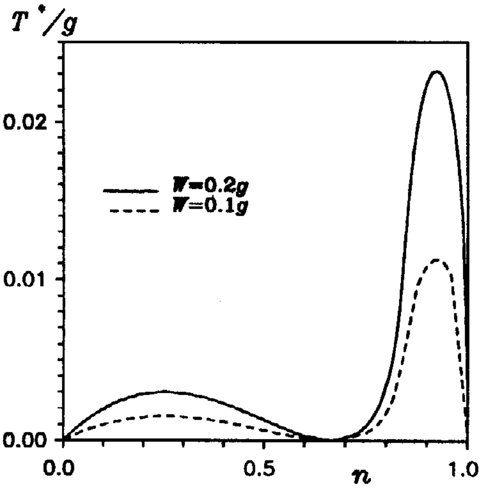

Figure 8: Dependence of the temperature of dielectric instability T^* on electron concentration n ($U \to \infty$, $\Omega = 0$, $h/g = 1.05$).

especially the anomalies of this function can initiate the transition to superconducting phase. The analogy (may be formal) between the right part of diagram $T^*(n)$ (fig. 8) and characteristic dependency of temperature T_c vs electron concentration in high-temperature superconductors can lead to this conclusion.

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A Matrices $\Pi''^{,\uparrow}_{(0)}$ and $\Pi''^{,\downarrow}_{(0)}$

$$\Pi''^{,\sigma} = \begin{pmatrix} \pi''^{,\sigma}_{aa} & \pi''^{,\sigma}_{ab} \\ \pi''^{,\sigma}_{ba} & \pi''^{,\sigma}_{bb} \end{pmatrix}, \tag{A.1}$$

where

$$\pi''^{,\uparrow}_{aa} = \begin{pmatrix} -\Phi''(41) & \Psi''(41,23) & -\Psi''(41,23) & \Phi''(41) \\ \Psi''(23,41) & -\Phi''(23) & \Phi''(23) & -\Psi''(23,41) \\ -\Psi''(23,41) & \Phi''(23) & -\Phi''(23) & \Psi''(23,41) \\ \Phi''(41) & -\Psi''(41,23) & \Psi''(41,23) & -\Phi''(41) \end{pmatrix},$$

$$\pi''^{,\uparrow}_{ab} = \begin{pmatrix} -\Psi''(41,\tilde{4}\tilde{1}) & \Psi''(41,\tilde{2}\tilde{3}) & -\Psi''(41,\tilde{2}\tilde{3}) & \Psi''(41,\tilde{4}\tilde{1}) \\ \Psi''(23,\tilde{4}\tilde{1}) & -\Psi''(23,\tilde{2}\tilde{3}) & \Psi''(23,\tilde{2}\tilde{3}) & -\Psi''(23,\tilde{4}\tilde{1}) \\ -\Psi''(23,\tilde{4}\tilde{1}) & \Psi''(23,\tilde{2}\tilde{3}) & -\Psi''(23,\tilde{2}\tilde{3}) & \Psi''(23,\tilde{4}\tilde{1}) \\ \Psi''(41,\tilde{4}\tilde{1}) & -\Psi''(41,\tilde{2}\tilde{3}) & \Psi''(41,\tilde{2}\tilde{3}) & -\Psi''(41,\tilde{4}\tilde{1}) \end{pmatrix},$$

$$\pi''^{,\downarrow}_{aa} = \begin{pmatrix} -\Phi''(31) & \Psi''(31,24) & \Phi''(31) & -\Psi''(31,24) \\ \Psi''(24,31) & -\Phi''(24) & -\Psi''(24,31) & \Phi''(24) \\ \Phi''(31) & -\Psi''(31,24) & -\Phi''(31) & \Psi''(31,24) \\ -\Psi''(24,31) & \Phi''(24) & \Psi''(24,31) & -\Phi''(24) \end{pmatrix},$$

$$\begin{aligned}
\pi''^{,\downarrow}_{ab} &= \begin{pmatrix} -\Psi''(31,\tilde{3}\tilde{1}) & \Psi''(31,\tilde{2}\tilde{4}) & \Psi''(31,\tilde{3}\tilde{1}) & -\Psi''(31,\tilde{2}\tilde{4}) \\ \Psi''(24,\tilde{3}\tilde{1}) & -\Psi''(24,\tilde{2}\tilde{4}) & -\Psi''(24,\tilde{3}\tilde{1}) & \Psi''(24,\tilde{2}\tilde{4}) \\ \Psi''(31,\tilde{3}\tilde{1}) & -\Psi''(31,\tilde{2}\tilde{4}) & -\Psi''(31,\tilde{3}\tilde{1}) & \Psi''(31,\tilde{2}\tilde{4}) \\ -\Psi''(24,\tilde{3}\tilde{1}) & \Psi''(24,\tilde{2}\tilde{4}) & \Psi''(24,\tilde{3}\tilde{1}) & -\Psi''(24,\tilde{2}\tilde{4}) \end{pmatrix}, \\
\pi''^{,\sigma}_{ba} &= \pi''^{,\sigma}_{ab}\left[(1,2,3,4) \rightleftharpoons \left(\tilde{1},\tilde{2},\tilde{3},\tilde{4}\right)\right], \qquad \text{(A.2)} \\
\pi''^{,\sigma}_{bb} &= \pi''^{,\sigma}_{aa}\left[(1,2,3,4) \rightleftharpoons \left(\tilde{1},\tilde{2},\tilde{3},\tilde{4}\right)\right].
\end{aligned}$$

B Dynamic dielectric susceptibility at $\mu = \text{const}$ and $n = \text{const}$

Let us consider the response of the system to the external electric field. The interaction with the field is taken into account adding term

$$H' = -E_{\perp} \sum_i P_i \qquad \text{(B.1)}$$

to the Hamiltonian, where

$$P_i = d_S S_i^z + d_e n_i \qquad \text{(B.2)}$$

is the variable part of the dipole momentum of the primitive cell consisting of ion and electron components. Formula (B.2) for the P_i vector corresponds to the consideration of the so-called transverse component of polarization. When the model is applied to the description of HTSC with layered structure of YBaCuO–type, this component is connected with the oxygen motions in the double–well potential along the direction normal to the Cu–O layer and with electron charge redistribution between layers and other structure elements [9].

Statistical operator of the system for the case of grand canonical ensemble $\hat{\rho} = e^{-\beta\mathcal{H}}$ is written as

$$\hat{\rho} = \exp\left\{-\beta\left[H - \sum_i \left(d_S S_i^z + d_e n_i\right) E_{\perp} - \mu \sum_i n_i\right]\right\}. \qquad \text{(B.3)}$$

In the interaction representation

$$\hat{\rho} = e^{-\beta H} T \exp\left\{\sum_i \int_0^\beta d\tau \left[P_i(\tau) E_{\perp} + \mu n_i(\tau)\right]\right\} \qquad \text{(B.4)}$$

we can generalize this expression introducing fictitious fields $h_i(\tau)$, $\mu_i(\tau)$

$$\hat{\rho} = e^{-\beta H} T \exp\left\{\sum_i \int_0^\beta d\tau \left[P_i(\tau) h_i(\tau) + n_i(\tau) \mu_i(\tau)\right]\right\} \qquad \text{(B.5)}$$

(at the end we shall put $h_i(\tau) \to E_{\perp}$; $\mu_i(\tau) \to \mu$). Obviously,

$$\frac{\delta Z}{\delta h_i(\tau)} = Z \left\langle P_i(\tau) \right\rangle; \qquad \frac{\delta Z}{\delta \mu_i(\tau)} = Z \left\langle n_i(\tau) \right\rangle, \qquad \text{(B.6)}$$

where $Z = \mathrm{Sp}\,\mathrm{e}^{-\beta\mathcal{H}}$ is the partition function.

We pass on to the momentum–frequency representation

$$f_i(\tau) = \frac{1}{\sqrt{N}} \sum_n \sum_{\mathbf{q}} f_{\mathbf{q}}(\bar{\omega}_n)\, \mathrm{e}^{i\bar{\omega}_n\tau} \mathrm{e}^{i\mathbf{q}\mathbf{R}_i} \tag{B.7}$$

(where $f_i = P_i$, h_i etc.). Then

$$\hat{\rho} = \mathrm{e}^{-\beta H} T \exp\left\{\beta \sum_{n\mathbf{q}} \left[P_{-\mathbf{q}}(-\bar{\omega}_n)\, h_{\mathbf{q}}(\bar{\omega}_n) + n_{-\mathbf{q}}(-\bar{\omega}_n)\, \mu_{\mathbf{q}}(\bar{\omega}_n)\right]\right\} \tag{B.8}$$

with

$$P_{\mathbf{q}}(\bar{\omega}_n) = d_S S_{\mathbf{q}}(\bar{\omega}_n) + d_e n_{\mathbf{q}}(\bar{\omega}_n). \tag{B.9}$$

The relations (B.6) take the form

$$\frac{\delta Z}{\delta h_{\mathbf{q}}(\bar{\omega}_n)} = \beta Z \langle P_{-\mathbf{q}}(-\bar{\omega}_n)\rangle; \qquad \frac{\delta Z}{\delta \mu_{\mathbf{q}}(\bar{\omega}_n)} = \beta Z \langle n_{-\mathbf{q}}(-\bar{\omega}_n)\rangle. \tag{B.10}$$

Functional derivative

$$\frac{\delta\langle P_i(\tau)\rangle}{\delta h_j(\tau_1)} = \langle T P_i(\tau) P_j(\tau_1)\rangle_c \equiv \chi_{ij}^{PP}(\tau - \tau_1) \tag{B.11}$$

determines the reaction of the system to the field $h_i(\tau)$. After the transformation (B.7) formula (B.11) takes the form

$$\begin{aligned}\frac{\delta\langle P_{-\mathbf{q}}(-\bar{\omega}_n)\rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} &= \beta \langle T P_{-\mathbf{q}}(-\bar{\omega}_n)\, P_{-\mathbf{q}'}(-\bar{\omega}_{n'})\rangle_c \equiv \\ &\delta(\mathbf{q}+\mathbf{q}')\,\delta(\bar{\omega}_n + \bar{\omega}_{n'})\, \chi_{-\mathbf{q}}^{PP}(-\bar{\omega}_n),\end{aligned} \tag{B.12}$$

where function χ^{PP} is the dynamic dielectric susceptibility of the system. Here we use the notation

$$\begin{aligned}\chi_{\mathbf{q}}^{AB}(\bar{\omega}_n) &= \int_0^\beta d(\tau-\tau') \sum_{i-j} \mathrm{e}^{-i\mathbf{q}(\mathbf{R}_i-\mathbf{R}_j)} \mathrm{e}^{-i\bar{\omega}_n(\tau-\tau')} \langle T A_i(\tau) B_j(\tau')\rangle_c = \\ &\beta \langle T A_{-\mathbf{q}}(-\bar{\omega}_n)\, B_{\mathbf{q}}(\bar{\omega}_n)\rangle_c\end{aligned} \tag{B.13}$$

for the Fourier–transform of the semi–invariant average of T–product of A_i and B_j.

The derivative with respect to field $h_j(\tau_1)$ in (B.11) is the partial one; fields $\mu_i(\tau)$ are supposed to be independent of variables $h_j(\tau_1)$. Hence, susceptibility $\chi_{\mathbf{q}}^{PP}(\bar{\omega}_n)$ describes dielectric response in regime $\mu = \mathrm{const}$.

Another situation takes place when the external field is applied to the system with constant number of particles. In this case, to ensure $n = \mathrm{const}$ regime the chemical potential value μ should be changed with the change of field $h_j(\tau)$. This means that we have to consider the derivative

$$\left.\frac{\delta\langle P_{-\mathbf{q}}(-\bar{\omega}_n)\rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})}\right|_{n=\mathrm{const}} = \frac{\delta\langle P_{-\mathbf{q}}(-\bar{\omega}_n)\rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} + \sum_{\mathbf{q}_1 n_1} \frac{\delta\langle P_{-\mathbf{q}}(-\bar{\omega}_n)\rangle}{\delta \mu_{\mathbf{q}_1}(\bar{\omega}_{n_1})} \cdot \frac{\delta \mu_{\mathbf{q}_1}(\bar{\omega}_{n_1})}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} \tag{B.14}$$

and determine $\delta\mu/\delta n$ from the conservation condition $\langle n_i \rangle = n$:

$$\delta \langle n_{\mathbf{q}} (\bar{\omega}_n) \rangle \delta(\mathbf{q}) \delta (\bar{\omega}_n) = 0, \tag{B.15}$$

that is from the equation

$$\left[\frac{\delta \langle n_{\mathbf{q}} (\bar{\omega}_n) \rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} + \sum_{\mathbf{q}_1 n_1} \frac{\delta \langle n_{\mathbf{q}} (\bar{\omega}_n) \rangle}{\delta \mu_{\mathbf{q}_1}(\bar{\omega}_{n_1})} \cdot \frac{\delta \mu_{\mathbf{q}_1} (\bar{\omega}_{n_1})}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} \right] \delta(\mathbf{q}) \delta (\bar{\omega}_n) = 0. \tag{B.16}$$

Since,

$$\begin{aligned} \frac{\delta \langle n_{\mathbf{q}} (\bar{\omega}_n) \rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} &= \beta \langle T n_{\mathbf{q}} (\bar{\omega}_n) P_{-\mathbf{q}'} (-\bar{\omega}_{n'}) \rangle_c \\ \frac{\delta \langle n_{\mathbf{q}} (\bar{\omega}_n) \rangle}{\delta \mu_{\mathbf{q}'}(\bar{\omega}_{n'})} &= \beta \langle T n_{\mathbf{q}} (\bar{\omega}_n) n_{-\mathbf{q}'} (-\bar{\omega}_{n'}) \rangle_c \end{aligned} \tag{B.17}$$

then, as it follows from (B.16),

$$\frac{\delta \mu_{\mathbf{q}} (\bar{\omega}_n)}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} = -\delta(\mathbf{q}) \delta(\mathbf{q}') \delta (\bar{\omega}_n) \delta (\bar{\omega}_{n'}) \left\{ \chi_{\mathbf{q}}^{nn} (\bar{\omega}_n) \right\}^{-1} \chi_{\mathbf{q}}^{nP} (\bar{\omega}_n). \tag{B.18}$$

We shall present derivative (B.14) in the same manner as (B.12)

$$\left. \frac{\delta \langle P_{-\mathbf{q}} (-\bar{\omega}_n) \rangle}{\delta h_{\mathbf{q}'}(\bar{\omega}_{n'})} \right|_{n=\mathrm{const}} = -\delta(\mathbf{q} + \mathbf{q}') \delta (\bar{\omega}_n + \bar{\omega}_{n'}) \tilde{\chi}_{-\mathbf{q}}^{PP} (-\bar{\omega}_n) \tag{B.19}$$

introducing susceptibility, which corresponds to the regime n = const. Substituting (B.18) into (B.14) with

$$\frac{\delta \langle P_{-\mathbf{q}} (-\bar{\omega}_n) \rangle}{\delta \mu_{\mathbf{q}'}(\bar{\omega}_{n'})} = \beta \langle T P_{-\mathbf{q}} (-\bar{\omega}_n) n_{-\mathbf{q}'} (-\bar{\omega}_{n'}) \rangle_c \tag{B.20}$$

we find

$$\tilde{\chi}_{\mathbf{q}}^{PP} (\bar{\omega}_n) - \chi_{\mathbf{q}}^{PP} (\bar{\omega}_n) = -\chi_{\mathbf{q}}^{Pn} (\bar{\omega}_n) \left\{ \chi_{\mathbf{q}}^{nn} (\bar{\omega}_n) \right\}^{-1} \chi_{\mathbf{q}}^{nP} (\bar{\omega}_n) \delta(\mathbf{q}) \delta (\bar{\omega}_n). \tag{B.21}$$

This relation provides the connection between dielectric susceptibilities corresponding to the regimes μ = const and n = const. We can separate ion, electron and mixed components in the total susceptibility using the expression (B.2) for the dipole momentum P_i in terms of pseudospin S_i^z and particle number n_i operators

$$\chi^{PP} = d_S^2 \chi^{SS} + d_e^2 \chi^{nn} + d_S d_e \left(\chi^{Sn} + \chi^{nS} \right). \tag{B.22}$$

It is clear that

$$\begin{aligned} \tilde{\chi}_0^{PP}(0) = d_S^2 \tilde{\chi}_0^{SS}(0) &= d_S^2 \left(\chi^{SS} - \frac{\chi^{Sn} \chi^{nS}}{\chi^{nn}} \right)_{0,0} \\ \tilde{\chi}_0^{nn}(0) = 0; \qquad & \tilde{\chi}_0^{Sn}(0) = \tilde{\chi}_0^{nS}(0) = 0. \end{aligned} \tag{B.23}$$

C Contributions from elementary loop diagrams at $\bar{\omega}_n \to 0$, $\mathbf{q} \to 0$

The analytical expressions corresponding to the elementary loop diagrams (zero–approximation loops) are given by the formulae (6.7), (6.12) and (6.17). In the $\bar{\omega}_n \to 0$, $\mathbf{q} \to 0$ limit (at $T = 0$) we have

$$
\begin{aligned}
&\frac{1}{N}\sum_{\mathbf{k}} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{k}+\mathbf{q})} \to \\
&\frac{1}{N}\sum_{\mathbf{k}} \lim_{\mathbf{q}\to 0} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})\right]}{B_{mr}\left(t_{\mathbf{k}} - t_{\mathbf{k}+\mathbf{q}}\right)} = \\
&\frac{1}{N}\sum_{\mathbf{k}} n'_+\left(\lambda_{mr} + B_{mr}t_{\mathbf{k}}\right) = -\frac{1}{N}\sum_{\mathbf{k}} \delta\left(\lambda_{mr} + B_{mr}t_{\mathbf{k}} - \mu\right) = \\
&\begin{cases} -\rho_{mr}(\mu) & \text{, if chemical potential is located in the } (mr) \text{ subband} \\ 0 & \text{, otherwise} \end{cases}
\end{aligned}
\tag{C.1}
$$

($\rho_{mr}(\mu)$ is the density of states of the (mr) subband at Fermi level, $n'_+(\lambda) = \frac{d}{d\lambda}n_+(\lambda)$);

$$
\begin{aligned}
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{k}+\mathbf{q})} \to \\
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}} n'_+\left(\lambda_{mr} + B_{mr}t_{\mathbf{k}}\right) = \\
&\begin{cases} -\frac{\mu}{B_{mr}}\rho_{mr}(\mu) & \text{, if chemical potential is located in the } (mr) \text{ subband} \\ 0 & \text{, otherwise} \end{cases} ;
\end{aligned}
\tag{C.2}
$$

$$
\begin{aligned}
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}} t_{\mathbf{k}+\mathbf{q}} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{mr}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{mr}(\mathbf{k}+\mathbf{q})} \to \\
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}}^2 n'_+\left(\lambda_{mr} + B_{mr}t_{\mathbf{k}}\right) = \\
&\begin{cases} -\left(\frac{\mu}{B_{mr}}\right)^2 \rho_{mr}(\mu) & \text{, if chemical potential is located in the } (mr) \text{ subband} \\ 0 & \text{, otherwise} \end{cases} ;
\end{aligned}
\tag{C.3}
$$

$$
\begin{aligned}
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}} t_{\mathbf{k}+\mathbf{q}} \frac{n_+\left[\varepsilon_{mr}(\mathbf{k})\right] - n_+\left[\varepsilon_{np}(\mathbf{k}+\mathbf{q})\right]}{i\bar{\omega}_n + \varepsilon_{mr}(\mathbf{k}) - \varepsilon_{np}(\mathbf{k}+\mathbf{q})} \to \\
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}}^2 \frac{1 - n_+\left(\varepsilon_{np}(\mathbf{k})\right)}{\varepsilon_{mr}(\mathbf{k}) - \varepsilon_{np}(\mathbf{k}+\mathbf{q})} \approx \\
&\frac{1}{N}\sum_{\mathbf{k}} t_{\mathbf{k}}^2 \frac{1 - n_+\left(\lambda_{np} + B_{np}t_{\mathbf{k}}\right)}{\lambda_{mr} - \lambda_{np}} = \frac{1}{\lambda_{mr} - \lambda_{np}} \cdot \frac{1}{6W}\left[W^3 - \left(\frac{\mu}{B_{np}}\right)^3\right]
\end{aligned}
\tag{C.4}
$$

(here $(mr) \neq (np)$; subband (mr) is completely filled, chemical potential is in the (np) subband).

We use the rectangular density of states

$$\rho_{np}(t) = \begin{cases} \frac{1}{2WB_{np}} & , -WB_{np} < t < WB_{np} \\ 0 & , t < -WB_{np}; \ t > WB_{np} \end{cases}, \tag{C.5}$$

where $2W$ is the width of the initial (uncorrelated) electron band; the origin of energy is at the band center.

Accordingly to (C.1)–(C.4), we have the following expressions for the components of the matrix $\hat{M}$:

1) $h > g$.

$$\begin{aligned} a = -\rho_{41}(\mu); \quad d = -\frac{\mu}{B_{41}}\rho_{41}(\mu); \quad \varphi = \left(\frac{\mu}{B_{41}}\right)^2 \rho_{41}(\mu), \\ \bar{f} = -\frac{B_{41}}{\lambda_{41} - \lambda_{\bar{4}\bar{1}}} \left(\frac{\mu}{B_{41}}\right)^2 \rho_{41}(\mu); \\ \psi = \frac{W^2}{6\left(\lambda_{41} - \lambda_{\bar{4}\bar{1}}\right)} \left[1 - \left(\frac{\mu}{B_{41}W}\right)^3\right]. \end{aligned} \tag{C.6}$$

Chemical potential is located within the subband (41); subband $(\tilde{4}\tilde{1})$ is completely filled ($\lambda_{41} - \lambda_{\bar{4}\bar{1}} = g > 0$).

2) $h < 0$.

$$\begin{aligned} b = -\rho_{\bar{4}\bar{1}}(\mu); \quad \bar{g} = -\frac{\mu}{B_{\bar{4}\bar{1}}}\rho_{\bar{4}\bar{1}}(\mu); \quad \bar{\varphi} = \left(\frac{\mu}{B_{\bar{4}\bar{1}}}\right)^2 \rho_{\bar{4}\bar{1}}(\mu), \\ f = \frac{B_{\bar{4}\bar{1}}}{\lambda_{41} - \lambda_{\bar{4}\bar{1}}} \left(\frac{\mu}{B_{\bar{4}\bar{1}}}\right)^2 \rho_{\bar{4}\bar{1}}(\mu); \\ \bar{\psi} = \frac{W^2}{6\left(\lambda_{41} - \lambda_{\bar{4}\bar{1}}\right)} \left[1 + \left(\frac{\mu}{B_{\bar{4}\bar{1}}W}\right)^3\right], \end{aligned} \tag{C.7}$$

chemical potential is within the subband $(\tilde{4}\tilde{1})$; subband (41) is empty.

3) $0 < h < g$.

$$\psi' = \frac{W^2}{3\left(\lambda_{41} - \lambda_{\bar{4}\bar{1}}\right)}, \tag{C.8}$$

subband $(\tilde{4}\tilde{1})$ is completely filled and subband (41) is empty; chemical potential is located between them.

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