



ІНСТИТУТ
ФІЗИКИ
КОНДЕНСОВАНИХ
СИСТЕМ

ICMP-98-34E

I.V.Stasyuk, T.S.Mysakovich

POLARIZABILITY OPERATOR FOR
PSEUDOSPIN-ELECTRON MODEL

УДК: 535.375.5

PACS: 72.10D, 72.10Di

Оператор поляризованості для псевдоспін-електронної моделі

І.В.Стасюк, Т.С.Мисакович

Анотація. Досліджено нефононні внески у комбінаційне розсіяння світла для псевдоспін-електронної моделі. Для побудови оператора поляризованості використовується мікроскопічний підхід і здійснюються операторні розклади в термінах операторів Хаббарда, використовуючи константу електронного переносу як формальний параметр розкладу. До розгляду приймалися два різні внески до дипольного моменту: один пов'язаний з негомеополарністю заповнення електронних станів на вузлах ґратки, інший - із дипольним моментом псевдоспінів.

Polarizability operator for pseudospin-electron model

I.V.Stasyuk, T.S.Mysakovich

Abstract. Nonphonon contributions to Raman light scattering are investigated for the pseudospin-electron model. To construct the polarizability operator, the microscopic approach is used, which is based on the operator expansion in terms of the Hubbard operators, using the electron transfer constant as a formal parameter of the expansion. Two different contributions to the dipole momentum are taken into account: one is connected with the nonhomeopolarity of filling of the electron states on a site, another - with the dipole momentum of the pseudospins.

1. Introduction

The problem of nonphonon contributions to Raman light scattering in the systems with the strong short-range Hubbard-type interaction between electrons remains a subject of interest in the last years in spite of the success achieved in the description of the magnetic and electron Raman scattering in the systems with antiferromagnetic ordering [1,2]. The approach used by [1,2] is based on some semiphenomenological assumptions to build the effective Hamiltonian of the interaction between a system and incident light. Fleury and Loudon ([1]) used this method for antiferromagnetics and Shastry and Shraiman ([2]) dealt with the Hubbard model.

The aim of this work is to investigate these contributions using the method which is based on the construction of a polarizability operator \hat{P} in the framework of a microscopic approach; the method was developed in [3–5]. This approach is applied to the case of the pseudospin-electron model. This model is believed to describe high-temperature superconductivity (the compounds of YBaCuO-type structure) and can be treated as the Hubbard model, including interactions with the local anharmonic vibrations.

To construct the \hat{P} -operator, the electron transfer parameter t is used as a formal expansion parameter. The expression for the polarizability operator \hat{P} in terms of the correlation functions built on the Hubbard operators are presented. Analysis of the achieved results is carried out.

2. General formulae

We start from the explicit expression for the cross-section of Raman light scattering ([3,4]):

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega_2} = \frac{1}{(4\pi \varepsilon_0)^2} \sqrt{\frac{\varepsilon_1}{\varepsilon_2}} \frac{\omega_2^3 \omega_1}{\hbar^2 c^4} \sum_{\alpha, \beta, \alpha', \beta'} e_{1\alpha} e_{2\beta} e_{1\alpha'} e_{2\beta'} H_{k_2, k_1}^{\beta' \alpha', \beta, \alpha}(\omega_1, \omega_2) \quad (1)$$

here \vec{e}_1, \vec{e}_2 are polarization vectors; ω_1, ω_2 are incident and scattered light frequencies; \vec{k}_1, \vec{k}_2 are corresponding wave vectors; $\varepsilon_{1,2} \equiv \varepsilon(\omega_1, \omega_2)$;

$H_{k_2, k_1}^{\beta' \alpha', \beta, \alpha}(\omega_1, \omega_2)$ is the Raman scattering tensor:

$$H_{k_2, -k_1; -k_2, k_1}^{\beta' \alpha', \beta, \alpha}(\omega_1, \omega_2) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i(\omega_1 - \omega_2)t} \times \quad (2)$$

$$\langle \hat{P}_{\vec{k}_2 - \vec{k}_1}^{\beta' \alpha'}(-\omega_1, t) \hat{P}_{-\vec{k}_2 \vec{k}_1}^{\beta \alpha}(\omega_1, 0) \rangle,$$

\hat{P} is the polarizability operator

$$\hat{P}_{\vec{k}', \vec{k}}^{\beta \alpha}(\omega, t) = - \int_{-\infty}^{+\infty} ds e^{i\omega(t-s)} \{ \{ \hat{M}^{\beta}(\vec{k}', t) | \hat{M}^{\alpha}(\vec{k}, s) \} \}, \quad (3)$$

here $\hat{M}^{\alpha}(\vec{k})$ is a dipole momentum of a crystal unit cell in the \vec{k} -representation and the symbol $\{ \{ \hat{M}^{\beta}(\vec{k}', t) | \hat{M}^{\alpha}(\vec{k}, s) \} \}$ stands for "unaveraged" Green's function defined in the following way ([5]):

$$\{ \{ A(t) | B(t') \} \} = -i \Theta(t - t') [A(t), B(t')]. \quad (4)$$

The equations of motion for this function have a form

$$\hbar \omega_1 \{ \{ A | B \} \}_{\omega_1, \omega_2} = \frac{\hbar}{2\pi} [A, B]_{\omega_1 - \omega_2} + \{ \{ [A, H] | B \} \}_{\omega_1, \omega_2}, \text{ or} \quad (5)$$

$$\hbar \omega_2 \{ \{ A | B \} \}_{\omega_1, \omega_2} = \frac{\hbar}{2\pi} [A, B]_{\omega_1 - \omega_2} - \{ \{ A | [B, H] \} \}_{\omega_1, \omega_2}. \quad (6)$$

It is used to construct the polarizability operator; the solutions of these equations are built in the form of operator series in powers of some parameters of a Hamiltonian. It has to be emphasized that this method does not use phenomenological assumptions.

3. The pseudospin-electron model

The Hamiltonian of the model has the following form [6] :

$$H = \sum_i H_i + \sum_{i,j,\sigma} t_{i,j} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma}, \quad (7)$$

here the Hamiltonian H_i describes the interaction with the local anharmonic vibrational modes, described by pseudospins:

$$H_i = U n_{i\uparrow} n_{i\downarrow} + E_0 (n_{i\uparrow} + n_{i\downarrow}) + g (n_{i\uparrow} + n_{i\downarrow}) S_i^z - \Omega S_i^x - h S_i^z, \quad (8)$$

$\hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma}$ are σ -spin electron creation and annihilation operators, $n_{\sigma,i} = \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i,\sigma}$ is the electron occupation number operator on the site i . The second term in (7) is responsible for the electron transfer from site to site. The single-site Hamiltonian H_i includes the on-site Coulomb repulsion of electrons with opposite spins (U -term), the on-site electron energy (E_0 -term), the interaction with the local vibrations (g -term), the splitting of the vibrational mode by tunneling (Ω -term), the asymmetry of the vibrational mode (h -term).

In the case of narrow electron bands ($t \ll U$), the single-site Hamiltonian H_i plays the role of a zero order approximation. Therefore let us consider the following single-site basis of states $|n_{i\uparrow}, n_{i\downarrow}, S_i^z\rangle$ ([6]):

$$\begin{aligned} |1\rangle &= |0, 0, \frac{1}{2}\rangle, |\tilde{1}\rangle = |0, 0, -\frac{1}{2}\rangle, \\ |2\rangle &= |1, 1, \frac{1}{2}\rangle, |\tilde{2}\rangle = |1, 1, -\frac{1}{2}\rangle, \\ |3\rangle &= |0, 1, \frac{1}{2}\rangle, |\tilde{3}\rangle = |0, 1, -\frac{1}{2}\rangle, \\ |4\rangle &= |1, 0, \frac{1}{2}\rangle, |\tilde{4}\rangle = |1, 0, -\frac{1}{2}\rangle. \end{aligned} \quad (9)$$

It is useful to introduce the Hubbard operators $X^{RS} = |R\rangle\langle S|$, acting in the space spanned by the vectors (9). The operators $\hat{c}_{i,\sigma}^\dagger, \hat{c}_{j,\sigma}, S_i^\alpha$ can be expressed in terms of the Hubbard operators:

$$\begin{aligned} \hat{c}_{i,\uparrow}^\dagger &= X_i^{41} + X_i^{23} + X_i^{\tilde{4}1} + X_i^{\tilde{2}3}, \hat{c}_{i,\downarrow}^\dagger = X_i^{31} - X_i^{24} + X_i^{\tilde{3}1} - X_i^{\tilde{2}4}, \\ \hat{c}_{j,\uparrow} &= X_i^{14} + X_i^{32} + X_i^{\tilde{1}4} + X_i^{\tilde{3}2}, \hat{c}_{i,\downarrow} = X_i^{13} - X_i^{42} + X_i^{\tilde{1}3} - X_i^{\tilde{4}2}, \\ S_i^z &= \frac{1}{2} \sum_R (X_i^{RR} - X_i^{\tilde{R}\tilde{R}}), S_i^x = \frac{1}{2} \sum_R (X_i^{R\tilde{R}} + X_i^{\tilde{R}R}). \end{aligned} \quad (10)$$

The expression for the Hamiltonian H_i can be written as follows:

$$\begin{aligned} H_i &= \frac{h}{2}(X_i^{\tilde{1}1} - X_i^{11}) + (E_0 + \frac{g-h}{2})(X_i^{33} + X_i^{44}) + \\ &+ (E_0 - \frac{g-h}{2})(X_i^{\tilde{3}3} + X_i^{\tilde{4}4}) + (2E_0 + U + \frac{2g-h}{2})X_i^{22} + \\ &+ (2E_0 + U - \frac{2g-h}{2})X_i^{\tilde{2}2} - \\ &- \frac{\Omega}{2}(X_i^{\tilde{1}1} + X_i^{\tilde{2}2} + X_i^{\tilde{3}3} + X_i^{\tilde{4}4} + X_i^{11} + X_i^{22} + X_i^{33} + X_i^{44}). \end{aligned} \quad (11)$$

Now let us reduce H_i to a diagonal form, using the transformation

$$\begin{aligned} |R\rangle &= \cos(\phi_r)|r\rangle + \sin(\phi_r)|\tilde{r}\rangle \\ |\tilde{R}\rangle &= \cos(\phi_r)|\tilde{r}\rangle - \sin(\phi_r)|r\rangle, \end{aligned} \quad (12)$$

where

$$\begin{aligned} \cos(2\phi_1) &= \frac{-h}{\sqrt{h^2 + \Omega^2}}, \cos(2\phi_2) = \frac{2g-h}{\sqrt{(2g-h)^2 + \Omega^2}}, \\ \cos(2\phi_3) &= \cos(2\phi_4) = \frac{g-h}{\sqrt{(g-h)^2 + \Omega^2}}. \end{aligned} \quad (13)$$

Thus we get for H_i in terms of the X^{rs} operators:

$$H_i = \sum_r \epsilon_r X_i^{rr}, \quad (14)$$

with

$$\begin{aligned} \epsilon_{1,\tilde{1}} &= \pm \frac{1}{2} \sqrt{h^2 + \Omega^2}, \epsilon_{2,\tilde{2}} = 2E_0 + U \pm \frac{1}{2} \sqrt{(2g-h)^2 + \Omega^2}, \\ \epsilon_{3,\tilde{3}} &= \epsilon_{3,\tilde{3}} = E_0 \pm \frac{1}{2} \sqrt{(g-h)^2 + \Omega^2}. \end{aligned} \quad (15)$$

The total Hamiltonian is given by the expression

$$H = \sum_{i,r} \epsilon_r X_i^{rr} + \sum_{i,j,\sigma} t_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}, \quad (16)$$

with

$$\begin{aligned} \hat{c}_{i,\uparrow}^\dagger &= \cos(\phi_4 - \phi_1)(X_i^{41} + X_i^{\tilde{4}1}) - \sin(\phi_4 - \phi_1)(X_i^{\tilde{4}1} - X_i^{41}) + \\ &+ \cos(\phi_2 - \phi_3)(X_i^{23} + X_i^{\tilde{2}3}) - \sin(\phi_2 - \phi_3)(X_i^{\tilde{2}3} - X_i^{23}), \\ \hat{c}_{i,\downarrow}^\dagger &= \cos(\phi_3 - \phi_1)(X_i^{31} + X_i^{\tilde{3}1}) - \sin(\phi_4 - \phi_1)(X_i^{\tilde{3}1} - X_i^{31}) - \\ &- \cos(\phi_2 - \phi_4)(X_i^{24} + X_i^{\tilde{2}4}) + \sin(\phi_2 - \phi_4)(X_i^{\tilde{2}4} - X_i^{24}). \end{aligned} \quad (17)$$

It was shown ([6]) that the electron spectrum of the pseudospin-electron model possesses eight subbands. The single-electron transitions energies

$$\epsilon_\nu = \epsilon_s - \epsilon_r, \quad (18)$$

where $\nu = (r, s) = (\tilde{1}4), (\tilde{1}4), (14), (\tilde{1}4), (\tilde{3}2), (\tilde{3}2), (32), (\tilde{3}2)$ are broadening into bands having a width of the order of t .

4. The polarizability operator

The dipole momentum of a unit cell is given by

$$M_i^\alpha = eR_i^\alpha (n_{\uparrow,i} + n_{\downarrow,i}) + \frac{d}{2} S_i^z, \quad (19)$$

or in terms of the X^{rs} operators

$$\begin{aligned} M_i^\alpha &= eR_i^\alpha (X_i^{22} + X_i^{\tilde{2}2} - X_i^{11} - X_i^{\tilde{1}1} + 1) + \\ &+ \frac{d}{2} \sum_r (\cos(2\phi_r)(X_i^{rr} - X_i^{\tilde{r}\tilde{r}}) + \sin(2\phi_r)(X_i^{\tilde{r}\tilde{r}} + X_i^{rr})), \end{aligned} \quad (20)$$

here the first term is connected with the nonhomeopolarity of filling of the electron states on a site, the second one is responsible for the dipole momentum of the pseudospins. To calculate unaveraged Green's function $\{\{M_k^\alpha|M_l^\beta\}\}$ we make an operator expansion, using t as a formal parameter of the expansion. At first we write the equation of motion, which is presented in the form (5):

$$\begin{aligned} \{\{M_k^\alpha|M_l^\beta\}\} &= \frac{\delta_{k,l}d^2}{4\hbar\omega_1} \sum_r \sin(4\phi_r)(X^{r\tilde{r}} - X^{\tilde{r}r}) + \quad (21) \\ &+ \sum_r \frac{\delta_{k,l}d^2}{4(\hbar\omega_1 - E_r + E_r^-)} (\sin(4\phi_r)X^{\tilde{r}r} - \sin^2(2\phi_r)(X^{rr} - X^{\tilde{r}r})) - \\ &- \sum_r \frac{\delta_{k,l}d^2}{4(\hbar\omega_1 + E_r - E_r^-)} (\sin(4\phi_r)X^{r\tilde{r}} - \sin^2(2\phi_r)(X^{rr} - X^{\tilde{r}r})) + \\ &+ \frac{eR_k^\alpha}{\hbar\omega_1} \sum_{i,j,\sigma} t_{i,j}(\delta_{i,k} - \delta_{j,k})\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}|\hat{M}_l^\beta\}\} + \\ &+ \sum_r \frac{d}{2\hbar\omega_1} \sum_{i,j,\sigma} t_{i,j} \cos(2\phi_r) \{\{[X^{rr} - X^{\tilde{r}r}, \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}]|\hat{M}_l^\beta\}\} + \\ &+ \sum_r \frac{d}{2(\hbar\omega_1 - E_r + E_r^-)} \sum_{i,j,\sigma} t_{i,j} \sin(2\phi_r) \{\{[X^{\tilde{r}r}, \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}]|\hat{M}_l^\beta\}\} + \\ &+ \sum_r \frac{d}{2(\hbar\omega_1 + E_r - E_r^-)} \sum_{i,j,\sigma} t_{i,j} \sin(2\phi_r) \{\{[X^{r\tilde{r}}, \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}]|\hat{M}_l^\beta\}\}. \end{aligned}$$

We can see that in contrast with the Hubbard and $t - J$ models (see [7]), for the case of the pseudospin-electron model Green's function $\{\{M_k^\alpha|M_l^\beta\}\}$ has the terms, which are of the zero order with respect to the electron transfer parameter. The appearance of these terms is caused by the pseudospin dipole momentum dynamics. Now we use for the function (20) the equation of motion in the form (6). The obtained after this procedure expression is very cumbersome, so we write out only one term of that:

$$\begin{aligned} \sum_{i,j,\sigma} t_{i,j}(\delta_{i,k} - \delta_{j,k})\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}|(n_{\uparrow l} + n_{\downarrow l})\}\} &= \quad (22) \\ \frac{1}{\hbar\omega_2} \sum_{\substack{i,j,\sigma \\ s,p,\sigma'}} t_{i,j}(\delta_{i,k} - \delta_{j,k})t_{s,p}(\delta_{p,l} - \delta_{s,l})\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}|\hat{c}_{s,\sigma'}^\dagger \hat{c}_{p,\sigma'}\}\} - \\ - \frac{1}{2\pi\omega_2} \sum_{i,j,\sigma} t_{i,j}(\delta_{i,k} - \delta_{j,k})(\delta_{i,l} - \delta_{j,l})\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}; \end{aligned}$$

the structure of other terms is similar. Then we again write the equation of motion in the form (6) in order to find Green's function $\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}|\hat{c}_{s,\sigma'}^\dagger \hat{c}_{p,\sigma'}\}\}$ up to the terms of the second order in t , considering the resonant term, which describes the one-electron transition $\tilde{1}4 \rightarrow 14$:

$$\begin{aligned} \sum_{\substack{i,j \\ s,p,\sigma'}} t_{i,j}(\delta_{i,k} - \delta_{j,k})t_{s,p}(\delta_{p,l} - \delta_{s,l})\cos^2(\phi_4 - \phi_1) \times \quad (23) \\ \{\{X_i^{\tilde{4}1} X_j^{14}|\hat{c}_{s,\sigma'}^\dagger \hat{c}_{p,\sigma'}\}\} = \\ \sum_{\substack{i,j \\ s,p}} \frac{t_{i,j}(\delta_{i,k} - \delta_{j,k})t_{s,p}(\delta_{p,l} - \delta_{s,l})\hbar\cos^2(\phi_4 - \phi_1)}{2\pi(\hbar\omega_1 - E_4 + E_1 + E_4^- - E_1^-)} \times \\ (X_i^{\tilde{4}1}(\cos(\phi_4 - \phi_1)(X_j^{11} + X_j^{44}) - \\ - \sin(\phi_4 - \phi_1)(X_j^{\tilde{1}1} - X_j^{\tilde{4}4}))\hat{c}_{s,\uparrow} - \\ - \hat{c}_{s,\uparrow}^{\tilde{4}1} X_i^{14}(\cos(\phi_4 - \phi_1)(X_j^{\tilde{1}1} + X_j^{\tilde{4}4})) - \\ - \sin(\phi_4 - \phi_1)(X_j^{\tilde{4}4} - X_j^{\tilde{1}1})) + \\ + X_i^{\tilde{4}1}(\cos(\phi_4 - \phi_1)(X_j^{34}) + \sin(\phi_4 - \phi_1)X_j^{\tilde{3}4})\hat{c}_{s,\downarrow} - \\ - \hat{c}_{s,\downarrow}^{\tilde{4}1} X_i^{14}(\cos(\phi_4 - \phi_1)(X_j^{\tilde{4}3}) - \sin(\phi_4 - \phi_1)X_j^{\tilde{4}3})). \end{aligned}$$

We have omitted in this expression the terms, connected with the doubly occupied states $|2 \rangle, |\tilde{2} \rangle$. If $i=s$, the expression can be written as follows:

$$\begin{aligned} \frac{\sum_{i,j} t_{i,j}^2(\delta_{i,k} - \delta_{j,k})(\delta_{j,l} - \delta_{i,l})\hbar\cos^2(\phi_4 - \phi_1)}{2\pi(\hbar\omega_1 - E_4 + E_1 + E_4^- - E_1^-)} \times \quad (24) \\ (\cos^2(\phi_4 - \phi_1)[X_i^{11}(X_j^{\tilde{4}4} + X_j^{\tilde{3}3}) - X_i^{\tilde{1}1}(X_j^{44} + X_j^{33})] - \\ - \sin(\phi_4 - \phi_1)\cos(\phi_4 - \phi_1)[(X_i^{\tilde{4}4} + X_i^{\tilde{3}3})(X_j^{11} + X_j^{\tilde{1}1}) + \\ + X_i^{\tilde{1}1}(X_j^{44} + X_j^{33} + X_j^{\tilde{4}4} + X_j^{\tilde{3}3})]. \end{aligned}$$

So we can see that the terms connected with the electron spin reorientation are absent in this expression because the subband $\tilde{1}4$ is created by the pseudospin dynamics - for the Hubbard model this subband is not present. This expression include the terms which effectively take into account the electron correlations on the neighbouring lattice sites in the connection with the pseudospin dynamics. The corresponding Raman scattering contributions can be important in the presence of the charge ordered states with the modulation of the electron density and pseu-

dospin orientation (the possibility of such ordering in the pseudospin-electron model with the unit cell doubling was investigated in [8]).

Let us consider the term, which is resonant at the transition $\tilde{1} \tilde{4} \rightarrow \tilde{3} \tilde{2}$:

$$\sum_{\substack{i,j, \\ s,p,\sigma'}} t_{i,j}(\delta_{i,k} - \delta_{j,k}) t_{s,p}(\delta_{p,l} - \delta_{s,l}) \cos(\phi_2 - \phi_3) \cos(\phi_4 - \phi_1) \times (25) \\ \{ \{ X_i^{41} X_j^{32} - X_i^{31} X_j^{42} | \hat{c}_{s,\sigma'}^\dagger \hat{c}_{p,\sigma'} \} \} = \\ \frac{\sum_{i,j} \hbar \cos(\phi_4 - \phi_1) \cos(\phi_2 - \phi_3) t_{i,j}(\delta_{i,k} - \delta_{j,k}) t_{s,j}(\delta_{j,l} - \delta_{s,l})}{2\pi(\hbar\omega_1 - E_{\tilde{1}} + E_{\tilde{4}} + E_{\tilde{3}} - E_{\tilde{2}})} \times \\ (X_i^{41} (\cos(\phi_2 - \phi_3) (X_j^{33} + \sin(\phi_2 - \phi_3) (X_j^{33}) \hat{c}_{s,\uparrow} - \\ - X_i^{41} (\cos(\phi_2 - \phi_3) (X_j^{34}) + \sin(\phi_2 - \phi_3) X_j^{34}) \hat{c}_{s,\downarrow}) + \\ + X_i^{31} (\cos(\phi_2 - \phi_3) (X_j^{44} + \sin(\phi_2 - \phi_3) (X_j^{44}) \hat{c}_{s,\downarrow} - \\ - X_i^{31} (\cos(\phi_2 - \phi_3) (X_j^{43} + \sin(\phi_2 - \phi_3) (X_j^{43}) \hat{c}_{s,\uparrow}),$$

having omitted the terms, including the states $|\tilde{2} \rangle, |\tilde{2} \rangle$. If $i=s$, we obtain the following formula:

$$\frac{\sum_{i,j} \hbar \cos(\phi_4 - \phi_1) \cos(\phi_2 - \phi_3) t_{i,j}^2 (\delta_{i,k} - \delta_{j,k}) (\delta_{j,l} - \delta_{i,l})}{2\pi(\hbar\omega_1 - E_{\tilde{1}} + E_{\tilde{4}} + E_{\tilde{3}} - E_{\tilde{2}})} \times (26) \\ [\cos(\phi_2 - \phi_3) \cos(\phi_4 - \phi_1) (X_i^{44} X_j^{33} + X_i^{33} X_j^{44} - X_i^{43} X_j^{34} - \\ - X_i^{34} X_j^{43}) + \sin(\phi_2 - \phi_3) \sin(\phi_4 - \phi_1) (X_i^{43} X_j^{34} + X_i^{34} X_j^{43} - \\ - X_i^{44} X_j^{33} - X_i^{33} X_j^{44}) + \sin(2\phi_4 - \phi_2 - \phi_1) X_i^{43} X_j^{34} + \\ + X_i^{43} X_j^{34} - X_i^{44} X_j^{33} - X_i^{33} X_j^{44}].$$

So we can see that there are present in this expression both the terms, connected with the reorientation of the electron spins and the ones, connected with the reorientation of the pseudospins. Therefore one can see that the Raman scattering at the transitions between bands, separated by U is connected with the electron spin dynamics, very similar to that described by Fleury and Loudon approach [1] (creation of magnon pairs), as well as with the pseudospin dynamics. To say something more definitely, we have to obtain and investigate the expression for the Raman scattering tensor. For this purpose Green's function $\langle\langle X^{rr} | X^{pp} \rangle\rangle$, $\langle\langle X^{rr} | X^{\tilde{p}\tilde{p}} \rangle\rangle$, $\langle\langle X^{rr} | X^{\tilde{p}p} \rangle\rangle$ and others have to be calculated - this investigation will be a subject of forthcoming publications.

5. Conclusions

The microscopic approach for the description of Raman light scattering was applied in this work for the pseudospin-electron model. The operator expansions in powers of the parameter of the electron hopping were carried out to calculate the polarizability operator. It was shown that the polarizability operator is not equal to zero if the electron hopping is absent, this is caused by the dipole transitions connected with the reorientation of pseudospins. Analysing the expression for the polarizability operator, we can see that there exist resonant transitions between the subbands of the pseudospin-electron model. Investigating the terms, which are proportional to t^2 we have shown that the two main scattering mechanisms can be separated between others. The first one is connected with the correlation of the pseudospin dynamics with the electron filling on the neighbouring sites, that can be important in the case of the charge and pseudospin spatial modulation. The second one is analogous to the two-magnon scattering in antiferromagnets which is here accompanied by the reorientation of pseudospins.

References

1. P. Fleury, R. Loudon, Scattering of light by one- and two-magnon excitations. Phys. Rev., 166, 514 (1968)
2. B.S. Shastry, B.I. Shraiman, Theory of Raman Scattering in Mott-Hubbard Systems Phys. Rev. Lett., 65, 1068 (1990)
3. R.A. Cowley, The lattice dynamics of an anharmonic crystal. Advances Phys., 12, 421 (1963)
4. R. Barry, I.W. Sharpe, Raman scattering from impurities in semiconductors. 1. General results. Can. J. Phys., 56, 550 (1978)
5. I.V. Stasyuk, Ya.I. Ivankiv, Raman scattering in crystals with ordering structure units // Preprint ITP-87-57P, Institute for Theoretical Physics, Kyiv (1987)
6. I.V. Stasyuk, A.M. Shvaika, On the electron spectrum of the Hubbard model including interactions with local anharmonicity vibrations. Phys. C, 213, 57 (1993)
7. I.V. Stasyuk, T.S. Mysakovich, Raman scattering tensor for Hubbard and $t - J$ models // Preprint ICMP-98-28E, Institute for Condensed Matter Physics, Lviv (1998)
8. I.V. Stasyuk, O.D. Danyliv, The account of effective interaction in the Hubbard model with local anharmonicity // Preprint ICMP-94-6Y, Institute for Condensed Matter Physics, Lviv (1994)

Препринти Інституту фізики конденсованих систем НАН України розповсюджуються серед наукових та інформаційних установ. Вони також доступні по електронній комп'ютерній мережі на WWW-сервері інституту за адресою <http://www.icmp.lviv.ua/>

The preprints of the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine are distributed to scientific and informational institutions. They also are available by computer network from Institute's WWW server (<http://www.icmp.lviv.ua/>)

Ігор Васильович Стасюк
Тарас Степанович Мисакович

ОПЕРАТОР ПОЛЯРИЗОВАНОСТІ ДЛЯ ПСЕВДОСПІН-ЕЛЕКТРОННОЇ
МОДЕЛІ

Роботу отримано 20 листопада 1998 р.

Затверджено до друку Вченою радою ІФКС НАН України

Рекомендовано до друку семінаром відділу квантової статистики

Виготовлено при ІФКС НАН України

© Усі права застережені