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RAMAN SCATTERING TENSOR FOR HUBBARD AND $t - J$
MODELS

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Тензор комбінаційного розсіяння світла для моделі Хаббарда і $t - J$ моделі

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Анотація. Досліджено нефононні внески у комбінаційне розсіяння світла для моделі Хаббарда і $t - J$ моделі. Для побудови оператора поляризованості використовується мікроскопічний підхід і здійснюються операторні розклади в термінах операторів Хаббарда, використовуючи t і J як формальні параметри розкладу. До розгляду приймалися два різні внески до дипольного моменту: один пов'язаний з негомеополарністю заповнення електронних станів на вузлах ґратки, інший - із дипольними переходами з основного у збуджені стани. З аналізу отриманого виразу для тензора розсіяння видно, що ці два механізми дають подібні внески. Досліджено вигляд тензора розсіяння в залежності від співвідношень між поляризацією падаючого і розсіяного світла.

Raman scattering tensor for Hubbard and $t - J$ models

I.V.Stasyuk, T.S.Mysakovich

Abstract. Nonphonon contributions to Raman light scattering are investigated for the Hubbard and $t - J$ models. To construct the polarisability operator the microscopic approach is used, which is based on the operator expansion in the terms of the Hubbard operators, using t and J as a formal parameters 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 transitions from the ground state to the excited ones. Analysing the expression for the scattering tensor, we can see that these two mechanisms give similar contributions. The dependence of the scattering intensity on the polarisation of the incident and scattered light is investigated.

1. Introduction

The investigation of Raman light scattering enable us to obtain the information about the low-frequency excitations in crystals. 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 cases of the Hubbard and $t - J$ models. To construct the \hat{P} -operator, the electron transfer parameter t and the effective exchange constant J are used as formal expansion parameters. The expressions for the polarizability operator \hat{P} in terms of the correlation functions built on the Hubbard operators are presented. Using these expressions, the formulae for the Raman scattering tensor are obtained for the cases of the Hubbard and $t - J$ models. 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 Hubbard model

First let us consider the case of the Hubbard model

$$\hat{H} = \sum_{i,j} t_{i,j} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \sum_i \mu \hat{n}_i. \quad (7)$$

We will restrict ourselves to the case of large U , so we can make expansion in powers of t/U at the construction of the \hat{P} -operator, considering only the terms which are linear and quadratic in t/U . In the case of the Hubbard model the dipole momentum has a form

$$\hat{M}_i = e \vec{R}_i (\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}). \quad (8)$$

Here the nonhomeopolarity of filling of the electron states on lattice sites is taken into account. It is useful to consider the following single-site basis of states $|n_{i,\downarrow}, n_{i,\uparrow}\rangle$

$$|1\rangle = |0, 0\rangle, |2\rangle = |1, 1\rangle, |3\rangle = |1, 0\rangle, |4\rangle = |0, 1\rangle \quad (9)$$

and to introduce the Hubbard operators $X^{r,s} = |r \rangle \langle s|$.

To calculate Green's function $\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\}$ at first we write the equation of motion (5):

$$\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\} = \frac{eR_k^\alpha}{\hbar\omega_1} \sum_{i,j,\sigma} t_{i,j}(\delta_{i,k} - \delta_{j,k})\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} | \hat{M}_l^\beta\}\}. \quad (10)$$

Then we use the equation of motion, which is written in the form (6):

$$\begin{aligned} \{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} | \hat{M}_l^\beta\}\} &= [\frac{\hbar}{2\pi}(\delta_{j,l} - \delta_{i,l})\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} - \\ &- \sum_{s,p\sigma'} t_{s,p}(\delta_{s,l} - \delta_{p,l})\{\{\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} | \hat{c}_{s,\sigma'}^\dagger \hat{c}_{p,\sigma'}\}\}] \frac{eR_l^\beta}{\hbar\omega_2}. \end{aligned} \quad (11)$$

To calculate this function we again write the equation of motion (5) and neglect the terms which are proportional to t^3 . Using this scheme, the following expression for Green's function $\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\}$ is obtained

$$\begin{aligned} \{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\} &= [\sum_{i,j,\sigma} t_{i,j}(\delta_{i,k} - \delta_{j,k})(\delta_{j,l} - \delta_{i,l})\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \\ &+ \frac{1}{\hbar\omega_1 + U}\hat{A}^\dagger - \frac{1}{\hbar\omega_1 - U}\hat{A} + \frac{1}{\hbar\omega_1}(\hat{A} - \hat{A}^\dagger)] \frac{e^2 R_k^\alpha R_l^\beta}{2\pi\hbar\omega_1\omega_2}, \end{aligned} \quad (12)$$

here U plays the role of the energetic distance between two levels which are responsible for the scattering,

$$\begin{aligned} \hat{A} &= \sum_{i,j,s} t_{i,j}t_{s,j}(\delta_{i,k} - \delta_{j,k})(\delta_{j,l} - \delta_{s,l}) \times \\ &(X_i^{31}(X_j^{22} + X_j^{44})(X_s^{13} - X_s^{42}) + X_i^{41}(X_s^{31} - X_s^{24})X_j^{12} - \\ &-(X_s^{41} + X_s^{23})(X_j^{11} + X_j^{44})X_i^{32} + X_i^{41}X_j^{34}(X_s^{42} - X_s^{13}) + \\ &+ X_i^{41}(X_j^{33} + X_j^{22})(X_s^{32} + X_s^{14}) + X_j^{21}(X_s^{13} - X_s^{42})X_i^{32} - \\ &-(X_s^{31} - X_s^{24})X_j^{43}X_i^{32} - X_i^{31}X_j^{43}(X_s^{14} + X_s^{32}) - \\ &- X_i^{31}(X_s^{41} + X_s^{23})X_j^{12} + X_j^{21}(X_s^{14} + X_s^{32})X_i^{42} + \\ &+(X_s^{41} + X_s^{23})X_j^{34}X_i^{42} + (X_s^{31} - X_s^{24})(X_j^{11} + X_j^{33})X_i^{42}). \end{aligned} \quad (13)$$

Comparing with [2], we can see that some terms in our expression (when $i = s$, $n_{i,\uparrow} + n_{i,\downarrow} = 1$ and neglecting the state $|2 \rangle$) are the same as the scattering Hamiltonian obtained in [2]:

$$\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\} \sim \sum_{i,j} (\delta_{i,k} - \delta_{j,k})(\delta_{i,l} - \delta_{j,l}) \frac{t_{i,j}^2}{\hbar\omega_1 - U} \hat{S}_i^\alpha \hat{S}_j^\beta, \quad (14)$$

considering only the resonant term. However, there are some additional terms in (11) which are not presented in [2], these terms describe electron transitions between the next nearest neighbors.

Now let us calculate the scattering tensor. To deal with this expression we will use the following formula:

$$\langle \hat{A}(\omega_1 - \omega_2) \hat{B}(\omega'_1 - \omega_1) \rangle = \delta(\omega'_1 - \omega_2) \frac{2Im \langle \langle \hat{B} | \hat{A} \rangle \rangle_{\omega+i\epsilon}}{e^{\beta\hbar\omega} - 1} \Big|_{\omega=\omega_1-\omega_2} \quad (15)$$

In consequence we obtain the following expression for the scattering tensor:

$$\begin{aligned} H_{k_2, k_1}^{\beta' \alpha', \beta, \alpha}(\omega_1, \omega_2) &= \sum_{\substack{n, n', n_1, n'_1 \\ i, j, i_1, j_1}} e^{i(\vec{k}_2(\vec{R}_{n_i} - \vec{R}_{n_1 i_1}) - \vec{k}_1(\vec{R}_{n'_j} - \vec{R}_{n'_1 j_1}))} \\ &\times \frac{e^4 2Im \langle \langle \hat{A} | \hat{A}^\dagger \rangle \rangle_{\omega=\omega_1-\omega_2} R_{ni}^\alpha R_{n'_j}^{\beta'} R_{n_1 i_1}^\alpha R_{n'_1 j_1}^{\beta'}}{(e^{\beta\hbar\omega} - 1)\hbar\omega_1\omega_2(\hbar\omega_1 - U)^2}, \end{aligned} \quad (16)$$

considering only the resonant term. So we have to calculate Green's function $\langle \langle \hat{A} | \hat{A}^\dagger \rangle \rangle$ using the Hamiltonian of the Hubbard model. We will use a decoupling procedure for Fermi type operators:

$$\begin{aligned} \langle X^{pq}(t) X^{rs}(t) X^{mn} X^{pl} \rangle &\approx \langle X^{pq}(t) X^{pl} \rangle \langle X^{rs}(t) X^{mn} \rangle \pm \\ &\pm \langle X^{pq}(t) X^{mn} \rangle \langle X^{rs}(t) X^{pl} \rangle, \end{aligned} \quad (17)$$

having split Boson operators X^{pp} in the product of two Fermi operators: $X^{pp} = X^{p1} X^{1p}$. When calculating Green's function $\langle \langle X^{pq} | X^{rs} \rangle \rangle$ (now X^{pq}, X^{rs} are Fermi operators), we use the Hubbard-1 approximation and neglect the state $|2 \rangle$. After some tedious algebra we obtain the following result:

$$\begin{aligned} H_{k_2, k_1}^{\beta' \alpha', \beta, \alpha}(\omega_1, \omega_2) &= \frac{\langle X^{11} + X^{33} \rangle^4}{N^2 \omega_1 \omega_2 (\hbar\omega_1 - U)^2} \times \\ &\sum_{q_1, q_2, q_3, q} \frac{\delta(k_2 - k_1 - q_1 + q + q_2 - q_3)}{(e^{\beta(\mu - \langle X^{11} + X^{33} \rangle t(q))} + 1)(e^{-\beta(\mu - \langle X^{11} + X^{33} \rangle t(q_1))} + 1)} \times \\ &\frac{\delta(\omega - \frac{\langle X^{11} + X^{33} \rangle}{\hbar}(t(q_1) - t(q) + t(q_3) - t(q_2)))}{(e^{\beta(\mu - \langle X^{11} + X^{33} \rangle t(q_2))} + 1)(e^{-\beta(\mu - \langle X^{11} + X^{33} \rangle t(q_3))} + 1)} \times \\ &\sin(q^\alpha)' (\sin(q_1^\beta) + \sin(q_3^\beta)) \sin(q_1^{\beta'}) (\sin(q^\alpha) + \sin(q_1^\alpha)) \end{aligned} \quad (18)$$

The equation for $\langle X^{11} + X^{33} \rangle$ can be written as follows:

$$2\langle X^{11} + X^{33} \rangle - 1 = \frac{1}{N} \sum_q \frac{\langle X^{11} + X^{33} \rangle}{e^{\beta(\mu - \langle X^{11} + X^{33} \rangle t(q))} + 1} \quad (19)$$

From the expression (18) we can see that the frequency of the scattered wave differs from that of the incident wave due to the two-electron transitions in the band - the integrand in (18) has a delta-peak at the frequency:

$$\begin{aligned}\omega &= \omega_1 - \omega_2 = \langle X^{11} + X^{33} \rangle [t(q_1) + t(q_3) - t(q_2) - t(q_3)], \\ q_1 + q_3 &= q_2 + q + k_2 - k_1.\end{aligned}\quad (20)$$

If we had replaced Boson operators X^{pp} by their mean value $\langle X^{pp} \rangle$, we would have obtained the one-electron transitions:

$$\omega_1 - \omega_2 = \langle X^{11} + X^{33} \rangle [t(q_1) - t(q)], \quad q_1 = q + k_2 - k_1. \quad (21)$$

This one-electron transitions also can be obtained from the nonresonant term in (12), which is linear in t . If we calculate the correlator $\langle X^{pp}(t)X^{qq} \rangle$ more precisely (using higher order approximations), we will obtain both the one-electron transitions and the two-electron transitions ([6]).

Calculating Green's function, we have used the Hubbard Hamiltonian with the excluded state $|2\rangle$, so we have obtained only the electron scattering. To consider the magnon scattering we will deal with the $t - J$ model.

4. The $t - J$ model

Now let us consider the case of nearly half filling $\langle n_{i,\uparrow} + n_{i,\downarrow} \rangle \approx 1$ and $U \gg t$. In this case the Hubbard Hamiltonian can be reduced to the effective Hamiltonian of the so-called $t - J$ model:

$$\hat{H}_{t-J} = \sum_{i,j,\sigma} t_{i,j} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} + \sum_{i,j} J_{i,j} (\hat{S}_i \hat{S}_j - \frac{\hat{n}_{i,\uparrow} \hat{n}_{j,\downarrow}}{4}) - \sum_i \mu \hat{n}_i, \quad (22)$$

here $\hat{c}_{i,\sigma}^\dagger = \hat{c}_{i,\sigma} (1 - \hat{n}_{i,-\sigma})$, $J = \frac{4t^2}{U}$. Let us add to this Hamiltonian some additional terms to consider excited states on the atoms ψ_{exc} , having different parity with respect to the ground state ϕ_0 and their interaction with the ground state:

$$\begin{aligned}\hat{H} &= \hat{H}_{t-J} + (E - \mu) \sum_{i,\sigma,\alpha} \hat{a}_{\alpha i,\sigma}^\dagger \hat{a}_{\alpha i,\sigma} + \\ &+ \sum_{i,j,\sigma,\alpha,\beta} M_{i,j}^{\alpha,\beta} (X_i^{31} X_j^{13} + X_i^{41} X_j^{14}) \hat{a}_{\alpha j,\sigma}^\dagger \hat{a}_{\beta i,\sigma}^\dagger -\end{aligned}\quad (23)$$

$$\begin{aligned}- \sum_{i,j,\alpha,\beta} K_{i,j}^{\alpha,\beta} (X_i^{33} \hat{a}_{\alpha j,\downarrow}^\dagger \hat{a}_{\beta j,\downarrow} + X_i^{44} \hat{a}_{\alpha j,\uparrow}^\dagger \hat{a}_{\beta j,\uparrow} + \\ + X_i^{34} \hat{a}_{\alpha j,\uparrow}^\dagger \hat{a}_{\beta j,\downarrow} + X_i^{43} \hat{a}_{\alpha j,\downarrow}^\dagger \hat{a}_{\beta j,\uparrow}),\end{aligned}$$

here E is the difference between the energy of the excited states and the one of the ground state. The terms, connected with $K_{i,j}^{\alpha,\beta}$, $M_{i,j}^{\alpha,\beta}$, describe exchange interaction between the ground and excited states. The dipole momentum has a form:

$$\hat{M}_i^\alpha = d^\alpha (\hat{a}_{\alpha i,\downarrow}^\dagger X_i^{13} + \hat{a}_{\alpha i,\uparrow}^\dagger X_i^{14} + h.c.) \quad (24)$$

We make expansion in terms of t/E , M/E , K/E at the construction of the polarizability operator, considering the linear terms in M/E , K/E and quadratic in t/E . The following formula for Green's function $\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\}$ is obtained:

$$\begin{aligned}\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\} &= \frac{\hbar e^2 d^\alpha d^\beta}{2\pi(\hbar\omega_1 - E)(\hbar\omega_2 - E)} \times \\ &[- \sum_i \delta_{k,l} \delta_{\alpha,\beta} t_{i,k} (X_i^{31} X_k^{13} + X_i^{41} X_k^{14}) - \\ &- \sum_i \delta_{k,l} 2J_{i,k} (\hat{S}_i \hat{S}_k - \frac{\hat{n}_i \hat{n}_k}{4}) \delta_{\alpha,\beta} - \\ &- M_{l,k}^{\alpha\beta} (X_k^{33} X_l^{33} + X_k^{44} X_l^{44} + X_k^{43} X_l^{34} + X_k^{34} X_l^{43}) - \\ &- \sum_i \delta_{l,k} K_{i,k}^{\alpha\beta} (X_k^{33} X_i^{33} + X_k^{44} X_i^{44} + X_k^{43} X_i^{34} + X_k^{34} X_i^{43})] + \\ &+ \frac{\hbar e^2 d^\alpha d^\beta \delta_{k,l} \delta_{\alpha,\beta}}{2\pi(\hbar\omega_1 - E)^2 (\hbar\omega_2 - E)} \sum_{i,j} t_{i,k} t_{j,k} (X_i^{31} X_j^{13} + X_i^{41} X_j^{14}).\end{aligned}\quad (25)$$

Here we consider only the resonant terms and $d^\alpha = \langle \phi_0 | r^\alpha | \psi_{exc} \rangle$. We have also eliminated in (25) the terms including the operators connected with the higher energetic states. The obtained expression for $\{\{\hat{M}_k^\alpha | \hat{M}_l^\beta\}\}$ is similar to that obtained in [1] for antiferromagnetics. The formula transforms into the simple product of spin operators $\hat{S}_i \hat{S}_j$ for the case of homeopolarity: $n_{i,\uparrow} + n_{i,\downarrow} = 1$ (the hole doping level is equal to zero) and the terms which are linear and quadratic in t/E arise from the pure band transitions.

Let us calculate the scattering tensor. A spin polaron approach can be used for the $t - J$ model in the region of small hole concentrations [7,8]. We introduce for electron operators $\hat{c}_{i,\sigma}$ the following representation on

two sublattices with spin up ($i \in \uparrow$) and spin down ($i \in \downarrow$):

$$\hat{c}_{i,\uparrow} = \hat{h}_i^\dagger, \hat{c}_{i,\downarrow} = \hat{h}_i^\dagger \hat{S}_i^+ (i \in \uparrow); \hat{c}_{i,\downarrow} = \hat{f}_i^\dagger, \hat{c}_{i,\uparrow} = \hat{f}_i^\dagger \hat{S}_i^- (i \in \downarrow), \quad (26)$$

here \hat{h}_i is a hole spinless operator and \hat{S}_i^\pm are spin operators. Employing the linear spin-wave approximation, we can write

$$S_i^\pm \approx b_{i1} (i \in \uparrow), S_i^\pm \approx b_{i2}^+ (i \in \downarrow); \quad (27)$$

b_{i1}, b_{i2} are magnon operators on two sublattices. Performing the canonical transformation for the Fourier components

$$b_{k1} = v_k \alpha_k + u_k \beta_{-k}^+, b_{k2} = v_k \beta_k + u_k \alpha_{-k}^+, \quad (28)$$

we obtain the following Hamiltonian of the spin polaron model:

$$H_{t-J} = \sum_k q (h_k^+ f_{k-q} [g(k, q) \alpha_q + g(q - k, q) \beta_q^+] + h.c.) - (29) \\ - \mu \sum_k (h_k^+ h_k + f_k^+ f_k) + \sum_q \omega_q (\alpha_q^+ \alpha_q + \beta_q^+ \beta_q).$$

Here

$$g(k, q) = 4t / \sqrt{N/2} (u_q \gamma_{k-q} + v_q \gamma_k), u_k = \sqrt{(1 + \nu_k) / 2\nu}, \quad (30) \\ v_k = -\text{sign}(\gamma_k) \sqrt{(1 - \nu_k) / 2\nu}, \nu_k = \sqrt{1 - \gamma_k^2}, \\ \gamma_k = 1/4 \sum_r e^{ikr}, \omega_k = 2J(1 - \delta)^2 \nu_k, \\ \delta = \langle h^+ h \rangle + \langle f^+ f \rangle. \quad (31)$$

This representation excludes doubly occupied states and takes into account strong antiferromagnetic spin correlations at the electron hopping. To simplify the calculations we will consider only the last diagonal term in the Hamiltonian.

Now we have to rewrite the Raman scattering tensor in terms of the hole spinless operators and the magnon operators:

$$H_{k_1, k_2}^{\beta' \alpha', \beta \alpha}(\omega_1, \omega_2) = \frac{e^4 \hbar^2 d^\alpha d^{\alpha'} d^\beta d^{\beta'} 2Im \langle \langle T_{n_1 i_1, n_1' j_1}^{\alpha \beta} | T_{n_1 i_1, n_1' j_1}^{\alpha' \beta'} \rangle \rangle}{(e^{\beta \hbar \omega} - 1)(\hbar \omega_1 - E)^2 (\hbar \omega_2 - E)^2}, \quad (32)$$

here the operator $T_{n_1 i_1, n_1' j_1}^{\alpha \beta}$ has a form:

$$T_{n_1 i_1, n_1' j_1}^{\alpha \beta} = [\delta_{\alpha \beta} \delta_{n_1 n_1'} \delta_{i_1 j_1} \sum_{m, l} 2J_{ml, n_1 i_1} (b_{ml} b_{n_1 i_1} + b_{ml}^+ b_{n_1 i_1}^+)] (33)$$

$$+ M_{n_1 i_1, n_1' j_1}^{\alpha \beta} (b_{n_1 i_1} b_{n_1' j_1} + b_{n_1' j_1}^+ b_{n_1 i_1}^+ + n_{n_1 i_1} + n_{n_1' j_1}) + \\ + \sum_{m, l} K_{n_1 i_1, ml}^{\alpha \beta} (b_{n_1 i_1} b_{ml} + b_{ml}^+ b_{n_1 i_1}^+ + n_{n_1 i_1} + n_{ml}) (1 - \delta)^2.$$

Here we consider the low values of magnon concentration and do not consider the term $n_i n_j$; we have also used the approximation: $h_i h_i^+ \rightarrow (1 - \delta)$. So we have to find Green's function built on the magnon operators, using the diagonal magnon Hamiltonian. For instance, let us calculate Green's function $\langle \langle b_{q1} b_{q2} | b_{q3}^+ b_{q4}^+ \rangle \rangle$. Using the above mentioned canonical transformation, we can write

$$\langle \langle b_{q1} b_{q2} | b_{q3}^+ b_{q4}^+ \rangle \rangle = \langle \langle \alpha_{q1} \alpha_{-q2}^+ | \alpha_{q3}^+ \alpha_{-q4} \rangle \rangle u_{q1} u_{q3} v_{q2} v_{q4} + (34) \\ + \langle \langle \beta_{-q1}^+ \beta_{q2} | \beta_{-q3} \beta_{q4}^+ \rangle \rangle u_{q2} u_{q4} v_{q1} v_{q3} + \\ + \langle \langle \alpha_{q1} \beta_{q2} | \alpha_{q3}^+ \beta_{q4}^+ \rangle \rangle u_{q1} u_{q3} u_{q2} u_{q4} + \\ + \langle \langle \beta_{-q1}^+ \alpha_{-q2} | \beta_{-q3} \alpha_{-q4} \rangle \rangle v_{q1} v_{q3} v_{q2} v_{q4}$$

The obtained functions can be easily calculated using the standard technique of the equations of motion:

$$\langle \langle \alpha_{q1} \alpha_{-q2}^+ | \alpha_{q3}^+ \alpha_{-q4} \rangle \rangle = \frac{\hbar}{2\pi} \delta_{q_1 q_3} \delta_{q_2 q_4} \frac{\langle n_{q_2} - n_{q_1} \rangle}{\hbar \omega - \omega_{q_1} + \omega_{q_2}} \quad (35)$$

$$\langle \langle \beta_{-q1}^+ \beta_{q2} | \beta_{-q3} \beta_{q4}^+ \rangle \rangle = \frac{\hbar}{2\pi} \delta_{q_1 q_3} \delta_{q_2 q_4} \frac{\langle n_{q_1} - n_{q_2} \rangle}{\hbar \omega + \omega_{q_1} - \omega_{q_2}}. \quad (36)$$

$$\langle \langle \alpha_{q1} \beta_{q2} | \alpha_{q3}^+ \beta_{q4}^+ \rangle \rangle = \frac{\hbar}{2\pi} \delta_{q_1 q_3} \delta_{q_2 q_4} \frac{\langle n_{q_2} + 1 + n_{q_1} \rangle}{\hbar \omega - \omega_{q_1} - \omega_{q_2}}. \quad (37)$$

$$\langle \langle \beta_{-q1}^+ \alpha_{-q2}^+ | \beta_{-q3} \alpha_{-q4} \rangle \rangle = -\frac{\hbar}{2\pi} \delta_{q_1 q_3} \delta_{q_2 q_4} \frac{\langle n_{q_2} + 1 + n_{q_1} \rangle}{\hbar \omega + \omega_{q_1} + \omega_{q_2}}, \quad (38)$$

$$\omega = \omega_1 - \omega_2.$$

By analogy with this Green's functions we can find all other functions. Considering a two-dimensional volume centered lattice, we can write the diagonal components of the scattering tensor as follows:

$$H^{xx;yy}(\omega_1, \omega_2) = \frac{(1 - \delta)^4 2\pi e^4 \hbar^2 d^4}{(e^{\beta \hbar \omega} - 1)(\hbar \omega_1 - E)^2 (\hbar \omega_2 - E)^2} \times (39) \\ [\sum_k (v_k^2 + u_k^2)^2 \delta(\omega - 2\omega_k) \cos^2(k_y/2) \cos^2(k_x/2) \times \\ 64(M^{xx} + J + K^{xx})^2 (2n_k + 1) + \\ + \sum_k 4v_k^2 u_k^2 \delta(\omega - 2\omega_k) (M^{xx} + K^{xx})^2 (2n_k + 1)],$$

The nondiagonal components of the tensor have a form

$$H^{xy;xy}(\omega_1, \omega_2) = \frac{(1-\delta)^4 2\pi e^4 \hbar^2 d^4}{(e^{\beta\hbar\omega} - 1)(\hbar\omega_1 - E)^2(\hbar\omega_2 - E)^2} \times$$

$$\left[\sum_k (v_k^2 + u_k^2)^2 \delta(\omega - 2\omega_k) \sin^2(k_y/2) \sin^2(k_x/2) \times \right.$$

$$\left. 64(M^{xy} + K^{xy})^2 (2n_k + 1) \right]. \quad (40)$$

The main contribution comes from Green's function $\langle\langle S^+ S^- | S^+ S^- \rangle\rangle$; Green's function $\langle\langle S^+ S^- | S^z S^z \rangle\rangle$, $\langle\langle S^z S^z | S^+ S^- \rangle\rangle$ do not lead to new terms and give contribution only to the diagonal components of the tensor.

The obtained results are similar to that obtained for antiferromagnetics [1] but the condition of homeopolarity is not valid for the $t-J$ model and so the hole doping level is not equal to zero. It has led to the appearance of the factor $(1-\delta)^4$ in the expression for the scattering tensor. If we do not use the approximation $h_i h_i^\dagger \rightarrow (1-\delta)$, the influence of the hole doping on the scattering will be more complicated.

5. General case.

Now let us consider the Hubbard model, which includes the higher energetic states:

$$\hat{H} = \sum_{i,j} t_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \sum_i \mu \hat{n}_i +$$

$$+(E - \mu) \sum_{i,\nu} \hat{a}_{\nu i,\sigma}^\dagger \hat{a}_{\nu i,\sigma} + \sum_{i,\nu} M_{ij}^{\lambda\nu} \hat{a}_{\lambda j,\sigma'}^\dagger \hat{a}_{\nu i,\sigma'} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}$$
(41)

and the polarizability operator has a form:

$$P_i^\alpha = eR_i^\alpha [n_{\uparrow i} + n_{\downarrow i} + \sum_\lambda (n_{\lambda\uparrow i} + n_{\lambda\downarrow i})] + d^\alpha \sum_\sigma [a_{\alpha i\sigma}^+ c_{i\sigma} + h.c.]. \quad (42)$$

Here the operators c, n refer to the ground state, the operators a_λ, n_λ refer to the excited states. We do not consider the term connected with $K_{ij}^{\alpha\beta}$ because it does not lead to the new contributions to the scattering tensor in comparison with that obtained from the term connected with $M_{ij}^{\alpha\beta}$.

By analogy to the previous cases we can obtain the following expression for operator Green's function $\{\{M^\alpha | M^\beta\}\}$:

$$\{\{M_k^\alpha | M_l^\beta\}\} = \hbar \frac{e^2 d^\alpha d^\beta}{2\pi} \left[\frac{1}{(\hbar\omega_1 - E)(\hbar\omega_2 - E)} \delta_{\alpha,\beta} \times \right. \quad (43)$$

$$\left[- \sum_i \delta_{k,l} t_{i,k} (X_i^{31} X_k^{13} + X_i^{41} X_k^{14}) - \right.$$

$$\left. - M_{l,k} (X_k^{33} X_l^{33} + X_k^{44} X_l^{44} + X_k^{43} X_l^{34} + X_k^{34} X_l^{43}) \right] +$$

$$+ \frac{\hbar e^2 R_k^\alpha R_l^\beta}{2\pi \hbar^2 \omega_1 \omega_2} \sum_{i,j,s} t_{i,j} t_{s,j} (\delta_{i,k} - \delta_{j,k})(\delta_{j,l} - \delta_{s,l}) \times$$

$$(X_i^{31} X_j^{44} X_s^{13} + X_i^{41} X_j^{33} X_s^{14} - X_i^{41} X_j^{34} X_s^{13} - X_i^{31} X_j^{43} X_s^{14}) -$$

$$- \hbar \frac{e^2 d^\alpha d^\beta}{2\pi} \left(\frac{1}{(\hbar\omega_1 - E + U)(\hbar\omega_2 - E)(\hbar\omega_2 - E)} - \right.$$

$$\left. - \frac{1}{(\hbar\omega_1 + E - U)(\hbar\omega_1 + E)(\hbar\omega_2 + E)} \right) \delta_{kl} t_{ik} t_{jl} \times$$

$$(X_i^{31} X_j^{14} X_k^{43} + X_i^{41} X_j^{13} X_k^{34} - X_i^{41} X_j^{14} X_k^{33} - X_i^{31} X_j^{13} X_k^{44}) -$$

$$- 2\hbar \frac{e^2 d^\alpha d^\beta}{2\pi} \left(\frac{1}{(\hbar\omega_1 - E + U)(\hbar\omega_2 - E)(\hbar\omega_2 - E + U)} + \right.$$

$$\left. + \frac{1}{(\hbar\omega_1 + E - U)(\hbar\omega_2 + E - U)(\hbar\omega_1 + E)} \right) \delta_{kl} t_{ik} t_{jl} \times$$

$$(X_i^{31} X_j^{14} X_k^{43} + X_i^{41} X_j^{13} X_k^{34} - X_i^{41} X_j^{14} X_k^{33} - X_i^{31} X_j^{13} X_k^{44}).$$

So we can see that there are resonant terms with the frequencies:

$$\hbar\omega_1 = E; \hbar\omega_1 = U; \hbar\omega_1 = E - U; \hbar\omega_1 = U - E. \quad (44)$$

For the case of large $U (U \gg \hbar\omega - E)$ and $i = j$ one of the terms has a form:

$$J(\vec{S}\vec{S} - nn/4), \quad (45)$$

which is analogous to the term of Green's function $\{\{M_k^\alpha | M_l^\beta\}\}$ (25) obtained for the $t-J$ model.

Let us consider the first and the second resonant terms and use the diagonal magnon Hamiltonian to calculate Green's function. Then the formula for the diagonal components of the scattering tensor can be written as follows:

$$H^{\alpha\alpha, \alpha\alpha(\beta\beta, \beta\beta)}(\omega_1, \omega_2) = \frac{(1-\delta)^4 2\pi e^4 \hbar^2}{(e^{\beta\hbar\omega} - 1)} \times$$

$$\sum_k (v_k^2 + u_k^2)^2 \delta(\omega - 2\omega_k) \left(\cos^2(k_y/2) \cos^2(k_x/2) \times \right.$$

$$\left. \left[\frac{4d^{xx} M^{xx}}{(\hbar\omega_1 - E)(\hbar\omega_2 - E)} + \frac{2a^2 t^2}{\hbar\omega_1 \hbar\omega_2 (\hbar\omega_1 - U)} \right]^2 (2n_k + 1) + \right.$$

$$+ \sin^2(k_y/2) \sin^2(k_x/2) \sin^2(2\gamma) (2n_k + 1) \times \left[\frac{4d^{x^2} M^{xy}}{(\hbar\omega_1 - E)(\hbar\omega_2 - E)} + \frac{2a^2 t^2}{\hbar\omega_1 \hbar\omega_2 (\hbar\omega_1 - U)} \right]^2. \quad (46)$$

The components $H^{\alpha\alpha,\beta\beta}$, $H^{\beta\beta,\alpha\alpha}$ differ from $H^{\alpha\alpha,\alpha\alpha}$ only by the sign of the second term. The nondiagonal components can be written in the form:

$$H^{\alpha\beta,\alpha\beta(\beta\alpha,\beta\alpha)}(\omega_1, \omega_2) = 2\pi \frac{e^4 \hbar^2}{(e^{\beta\hbar\omega} - 1)} \sum_k (v_k^2 + u_k^2)^2 \times \delta(\omega - 2\omega_k) \left[\frac{4d^{x^2} M^{xy}}{(\hbar\omega_1 - E)(\hbar\omega_2 - E)} + \frac{2a^2 t^2}{\hbar\omega_1 \hbar\omega_2 (\hbar\omega_1 - U)} \right]^2 \times (2n_k + 1) \cos^2(2\gamma) \sin^2(k_y/2) \sin^2(k_x/2) (1 - \delta)^4. \quad (47)$$

Here γ is the angle between the crystal axes and the polarization axes (see fig. 1.). This angle is equal to zero in the previous cases. We can see

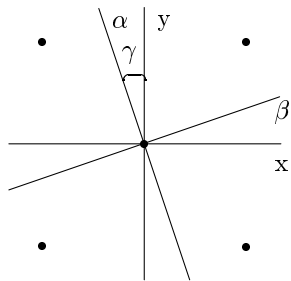


Figure 1. Dark filled circles depict atoms; x,y are crystal axes; α, β are polarization axes.

that if it is not so, the diagonal components of the tensor have the term which is proportional to $\sin(k_x/2)\sin(k_y/2)$; this term lead to the peak at the edge of the Brillouin zone ([1]).

6. Summary

The method of the construction of the polarizability operator for systems with the strong short-range correlation between electrons is developed in this work. The expressions for the polarizability operator in terms of the

correlation functions calculated on the Hubbard operators are obtained for the cases of the Hubbard and $t-J$ models. It is shown that in the case of the Hubbard model the frequency change is caused by the electron transitions in the band. In the case of the $t-J$ model the frequency change is due to the creation of the pair of magnons.

Two different contributions to the polarizability operator were taken into account, one is connected with the nonhomeopolarity of filling of the electron states on a site, another is responsible for the dipole transitions to the excited states. This two mechanisms lead to similar contributions to the scattering tensor. The comparison with the formulae derived in the framework of the method used in [1,2] is done. Using the obtained results we can investigate the electron and magnon contributions to Raman scattering in the systems with the strong short-range interaction between electrons and study the influence of the hole doping on this scattering.

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, A model with local anharmonicity in the theory of HTSC systems: correlation functions and "transverse" dielectric susceptibility, *Con.matt.phys.*, 1994, 3
7. N.M. Plakida, V.S. Oudovenko, and V.Yu. Yushankhai, Temperature and doping dependence of the quasiparticle spectrum for holes in the spin-polaron model of copper oxides. *Phys. Rev. B*, v.50, p.6431 (1994)
8. G. Martinez, P. Horsch, Spin-Polarons in the $t-J$ model. *Phys. Rev. B* v.44, p.317 (1991)

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ХАББАРДА І $t - J$ МОДЕЛІ

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