Національна академія наук України

ІНСТИТУТ
ФІЗИКИ
КОНДЕНСОВАНИХ
СИСТЕМ

ICMP–11–05E

R.Ya.Stetsiv, R.Ya.Yurechko*

DYNAMICAL CONDUCTIVITY
OF QUASI-ONE-DIMENSIONAL SYSTEMS
WITH HYDROGEN BONDS

Роман Ярославович Стеців
Роман Ярославович Юречко

Динамічна провідність квазіодновимірних систем з водневими зв'язками

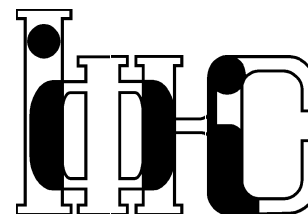*Lviv Polytechnic National University, 12 Bandera Str., 79013 Lviv, Ukraine

ЛЬВІВ

Динамічна провідність квазіодновимірних систем з водневими зв'язками

Р.Я.Стеців, Р.Я.Юречко

Анотація. На основі псевдоспін-електронної моделі досліджено частотну залежність динамічної провідності квазіодновимірних систем з водневими зв'язками. В моделі враховано протон-електронну взаємодію, зовнішнє поздовжнє поле h, тунелювання протонів, електронний транспорт і пряму протон-протонну взаємодію. Отримано залежність електронної концентрації і середньої заселеності протонних позицій від температури і поля h. Отримано лінію фазових переходів з однорідної фази до фази з модуляцією заряду. Досліджено залежність динамічної провідності від поля h і температури та її зміни при фазових переходах.

Dynamical conductivity of quasi-one-dimensional systems with hydrogen bonds

R.Ya.Stetsiv, R.Ya.Yurechko

Abstract. The frequency dependence of dynamical conductivity of the quasi-one-dimensional structures with hydrogen bonds is studies on the bases of pseudospin-electron model. It is taken into account the proton-electron interaction, external longitudinal field h, the tunneling hopping of protons, electron transfer and direct interaction between protons. The dependence of the electron concentration and mean number of protons on site on temperature and external field are obtained. The phase transition lines from uniform phase into charge ordered phase is determined. The dependence of the dynamical conductivity on temperature and field h and it changes at the phase transitions are obtained.

1. Introduction

The properties of the molecular and crystalline structures with hydrogen bonds is mainly determined by the character of protons redistribution on the bonds. We investigate the microscopic mechanisms of the charge transfer in a such systems on the basis of proposed pseudospin-electron model [1,2] that take into account correlation between the proton displacement and reconstruction of electron states as well as the change of their occupancy. This interaction is manifested itself as a cooperative proton-electron transfer (PET) in a series of experimental works [3–10] and it follows also from the results of quantum-chemical calculations [1,11–13]. Quantum chemical methods allow us to examine these charge redistributions in detail. The structural and optical studies of the proton transfer in N-salicylideneaniline [8,10] show that photochromism and thermochromism in these object arise from a proton transfer. The proton transfer accompanied by a configurational change of electron structure. It was shown that behaviour of proton dynamics is good consistent with the temperature dependence of visible absorption spectra of this crystal. If we could construct a molecular conductor based on this type of molecules, the charge transport might strongly be modulated by the proton motion. Photoinduced proton-coupled electron transfer (PCET) is investigated in a series of works [14–17] as one of the mechanisms of energy transformation in biological and chemical systems. Effect of a such proton-electron coupling plays an important role in passing a proton through the biological membrane in photosynthesis. The design and construction of a electron-proton hybrid system using the elements of 1-dimensional metal chains, acceptor (or donor) molecules, and interchain H-bonds is proposed [4]. A new molecular functions is expected to be produced in this system, if the motion of proton is closely correlated with the dynamics of the $1 - D$ electronic states. Similar effect is observed in the halogen (X)-bridge mixed-valence transition-metal (M) complexes ($M-X$-complexes) [3]. The $M-X$-complexes $[MA_2X]Y_2$ ($M = Pt, Pd$ or Ni) have a one-dimensional ($1D$)chain structure and adjacent chains are connected by hydrogen bonds. Here X stands for a bridging halogen ion ($X = Cl, Br$ or J), A for a ligand molecule (e.g. ethylenediamine, cyclohexenediamine), and Y for a counter anion (e.g. $Y = Br^-, ClO_4^-$). The location of the protons on $N - H - Y$ induce additional electron charges on the ions M and at some conditions they form the charge-ordered state (CDW) [3]. It is pointed out that the electron-proton coupling can control the CDW state [18].

We investigate the phase transition from uniform phase into charge-

ordered phase in a such system. In this work we study thermodynamic properties and the frequency dependence of dynamical conductivity of quasi-one-dimensional structures with hydrogen bonds on the bases of proposed pseudospin-electron model.

2. Hamiltonian

The Hamiltonian of quasi-one-dimensional structures which contains a chains with hydrogen bonds we write in the form [2]:

$$
\begin{aligned}
H_{eff} = &\sum_l \sum_{i,\sigma} ((\varepsilon - \mu) n_{i\sigma}(l) + g(n_{i\sigma}(l) - n_{i+1,\sigma}(l)) S_i^z(l)) + \\
&+ \sum_{l,l'} \sum_{i,j,\sigma} t_{i(l),j(l')}(a_{i\sigma}^+(l) a_{j,\sigma}(l') + a_{j,\sigma}^+(l') a_{i\sigma}(l)) + \\
&+ \sum_l \sum_i \Omega S_i^x(l) \\
&- \sum_l \sum_i h S_i^z(l) \\
&- \frac{1}{2} \sum_{l,l'} \sum_{i,j} J_{i(l),j(l')} S_i^z(l) S_j^z(l').
\end{aligned}
\tag{1}
$$

Here marked the summation along chains, indices i, j; and summation over chains indices l, l'. Pseudospin operator $\hat{S}_i$ describe the proton states in double potential well on the hydrogen bond. We consider the transfer along hydrogen bond is the dominant $t = t_{i(l),i+1(l)}$; $n_{i\sigma}$ – operator of electron concentration of i – position, σ – electron spin, μ – chemical potential of electrons.

The Hamiltonian includes proton-electron interaction (parameter g), electron transfer (parameter t), energy of proton tunneling (parameter Ω), asymmetry of the local anharmonic potential (parameter h). The last term describe proton-proton interaction.

Pseudospin-electron interaction forms the effective interaction between pseudospin (between protons in our case) and as it is shown in [19, 20], can cause the appearance of the modulated phase with doubling of the initial lattice period and can lead corresponding charge modulation. The study of this phenomenon is devoted this paper. In a double modulation of the lattice period the crystal is divided into two sublattice. We introduce the such designations: $\eta_\alpha = \langle S_{i,\alpha}^z \rangle$, $n_\alpha = \langle \sum_\sigma n_{i,\alpha,\sigma} \rangle$, ($\alpha = 1, 2$ is the sublattice index). In mean field approximation (MF) and pass-

ing to k-representation the Hamiltonian (1) has a form:

$$
H_{MF} = H_{el} + H_{sp} + U,
\tag{2}
$$

$$
H_{el} = \sum_{k,\alpha,\sigma} (\varepsilon - \mu + g(\eta_\alpha - \eta_\beta)) n_{k,\alpha,\sigma} + \sum_{k,\alpha,\sigma} t_{k,\alpha,\sigma} a_{k,\alpha,\sigma}^+ a_{k,\beta,\sigma}, \alpha \neq \beta,
$$

$$
t_k^{11} = t_k^{22} = 0, t_k \equiv t_k^{12} = t_k^{21} = \sum_{i(l)-j(l')} t_{i(l),j(l')}^{12} \, exp[i\vec{k}(\vec{R}_{i(l),1} - \vec{R}_{j(l'),2})],
$$

$$
H_{sp} = \sum_l \sum_{i,\alpha} (\Omega S_{i,\alpha}^x(l) - (h + j\eta_\beta - g(n_\alpha - n_\beta)) S_{i,\alpha}^z(l)),
$$

$$
U = \frac{1}{2} N j \eta_1 \eta_2 - \frac{N}{2} g(n_1 - n_2)(\eta_1 - \eta_2), \quad J = \sum_{l'} \sum_j J_{i(l),j(l')}.
$$

The electronic part of Hamiltonian (2) is diagonalized by unitary transformation

$$
a_{k,1,\sigma} = \tilde{a}_{k,1,\sigma} \cos \varphi + \tilde{a}_{k,2,\sigma} \sin \varphi,
\tag{3}
$$

$$
a_{k,2,\sigma} = -\tilde{a}_{k,1,\sigma} \sin \varphi + \tilde{a}_{k,2,\sigma} \cos \varphi,
$$

$$
\cos 2\varphi = \frac{-g(\eta_1 - \eta_2)}{\sqrt{g^2(\eta_1 - \eta_2)^2 + t_k^2}}, \sin 2\varphi = \frac{t_k}{\sqrt{g^2(\eta_1 - \eta_2)^2 + t_k^2}}
$$

In result we obtain:

$$
H_{el} = \sum_{k,\alpha,\sigma} (E_{k,\alpha} - \mu) \tilde{n}_{k,\alpha,\sigma},
\tag{4}
$$

$$
E_{k,\alpha} = \varepsilon + (-1)^\alpha \sqrt{g^2(\eta_1 - \eta_2)^2 + t_k^2}.
$$

The spin part of Hamiltonian is diagonalized by unitary transformation:

$$
\begin{aligned}
S_i^x(l) &= \tilde{S}_i^x(l) \cos \psi + \tilde{S}_i^z(l) \sin \psi, \\
S_i^z(l) &= -\tilde{S}_i^x(l) \sin \psi + \tilde{S}_i^z(l) \cos \psi, \\
\cos \psi_\alpha &= (h + j\eta_\beta - g(n_\alpha - n_\beta))/\lambda_\alpha, \sin \psi_\alpha = \Omega/\lambda_\alpha.
\end{aligned}
$$

In result we obtain:

$$
H_{sp} = -\sum_l \sum_{i,\alpha} \lambda_\alpha \tilde{S}_{i,\alpha}^z(l),
\tag{5}
$$

$$
\lambda_\alpha = \sqrt{(h + j\eta_\beta - g(n_\alpha - n_\beta))^2 + \Omega^2}.
$$

3. Thermodynamic properties

We obtain the equations for electron concentration n_α and average mean of pseudospins η_α in sublattices using (2) - (5):

$$n_\alpha = \frac{1}{\frac{N}{2}} \sum_{k,\alpha,\sigma} \left(\frac{1 + \cos 2\varphi}{2} (1 + \exp[\beta(E_{k,\alpha} - \mu)])^{-1} + \right.$$

$$\left. \frac{1 - \cos 2\varphi}{2} (1 + \exp[\beta(E_{k,\beta} - \mu)])^{-1} \right), \qquad (6)$$

$$\eta_\alpha = \frac{h + j\eta_\beta - g(n_\alpha - n_\beta)}{2\lambda_\alpha} th\left(\frac{\lambda_\alpha}{2kT} \right). \qquad (7)$$

From all the possible solutions of equations (6) - (7) choose the ones that give minimum Thermodynamic potential Φ in regime of $\mu = const$ or minimum of Free energy $F = \Phi + \mu N$ in regime $n = const$. Thermodynamic potential in MF - approximation has a form:

$$\Phi = -2kT \sum_k \ln((1 + \exp[-\beta(E_{k,1} - \mu)])(1 + \exp[-\beta(E_{k,2} - \mu)])) -$$

$$\frac{1}{2}kTN \ln(4ch\left(\frac{\lambda_1}{2kT} \right) ch\left(\frac{\lambda_2}{2kT} \right)) +$$

$$\frac{1}{2}Nj\eta_1\eta_2 - \frac{1}{2}Ng(n_1 - n_2)(\eta_1 - \eta_2) \qquad (8)$$

From the relations (6)–(7) we obtain the expressions for $\delta n = n_1 - n_2$ and $\delta\eta = \eta_1 - \eta_2$, which can play a role of the order parameter for modulated phase. Using this expressions we have a next condition of the appearance of nonzero solutions for δn and $\delta\eta$, and equation for temperature of the second order phase transition to modulated phase.

$$\frac{2}{\lambda^2}\left(\frac{\Omega^2}{\lambda} \langle \sigma^z \rangle + \right.$$

$$\frac{1}{kT}(h + j\eta)^2 \left(\frac{1}{4} - \langle \sigma^z \rangle^2 \right) \right) \left(\frac{1}{2}j - \frac{4}{N} \sum_k \frac{g^2}{t_k} \delta\eta((1 + \exp[\beta(\varepsilon - |t_k| - \mu)])^{-1} -$$

$$(1 + \exp[\beta(\varepsilon + |t_k| - \mu)])^{-1})) + 1 = 0 \qquad (9)$$

Here:

$$n = \frac{n_1 + n_2}{2}, \eta = \frac{\eta_1 + \eta_2}{2}, \langle \sigma^z \rangle = \frac{1}{2}th\left(\frac{\lambda}{2kT} \right).$$

$$\lambda = \sqrt{(h + j\eta)^2 + \Omega^2}.$$

The phase transition lines of the first and second order from the uniform phase to the phase with double modulation are shown in Fig.1: (a) for different values of the chemical potential μ, (b) for different values of parameter j and for $\Omega = 0$ and $\Omega = 0.05eV$ cases. Transition point of the first kind defined by numerical calculation, as the point at which the requirement of minimum for thermodynamic potential of changing the parameters of the model is transition from a homogeneous solution $n_1 = n_2$, $\eta_1 = \eta_2$ to modulated with δn and $\delta\eta$ different from zero. The line of phase transitions of the second order are bold. The splitting of the electron band at phase transition is shown in Fig.2. The temperature dependence of a mean numbers of electrons of sublattice n_1, n_2, and uniform phase n_0 also, along the phase transition line are shown in Fig.3. The temperature dependence of a mean values of pseudospins η_1, η_2, η_0 are illustrated in Fig.3 also. The temperature dependence of $\delta n(T)$ i $\delta\eta(T)$ are illustrated in Fig.4. These results are obtained for the next values of parameters: $g = 0.08eV$, $t = 0.05eV$, $j = 0$, $\mu = 0$, $\Omega = 0$ and $\Omega = 0.05eV$. The results for $j \neq 0$, $\mu \neq 0$ are presented in Fig.1. A such choice the values of parameters is give in [1]. All energy characteristics are in eV units.

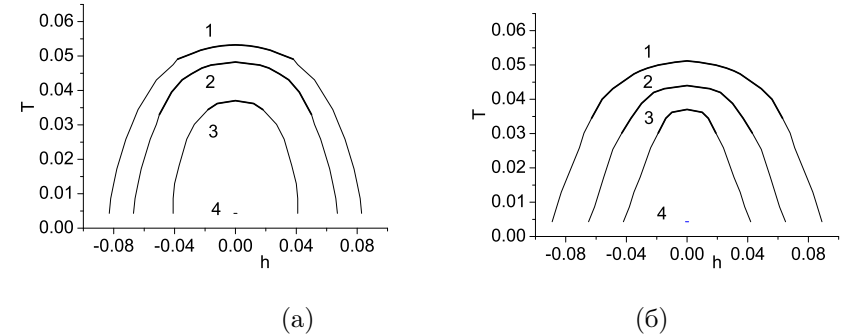(a)   (б)

Figure 1. The phase transition lines of the first and second order from the uniform phase to the phase with double modulation: (a) for for different values of the chemical potential μ: $1, 2, 3, 4 - \mu = 0, 0.05, 0.08, 0.12eV$ ($\Omega = 0$, $j = 0$), (b) for different values of parameter j: $1, 2, 3, 4 - j = 0, 0.05, 0.1, 0.2eV$ ($\Omega = 0.05eV$, $\mu = 0$).
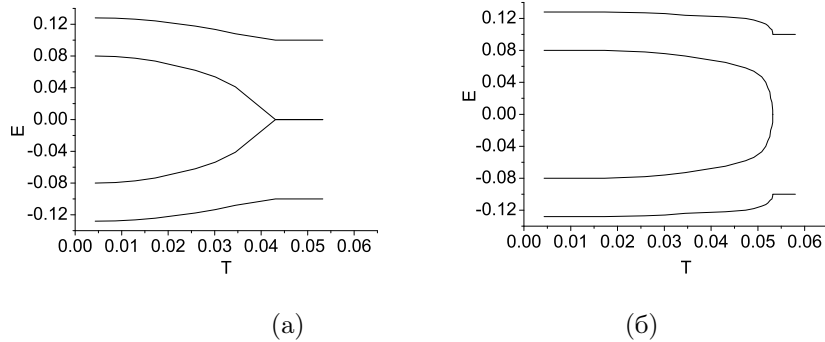
(a)　　　　　　　　　　　　　　(б)

Figure 2. The splitting of the electron band: (a) at phase transition along the phase transition line (b) for $h = 0$ in charge ordered phase $\Omega = 0$).
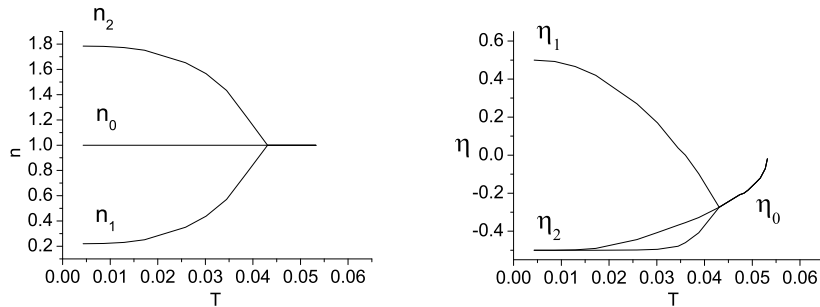

Figure 3. The temperature dependence of a mean numbers of electrons of sublattice n_1, n_2, and uniform phase n_0 and temperature dependence of a mean values of pseudospines η_1, η_2, η_0 along the phase transition line, $\Omega = 0$.
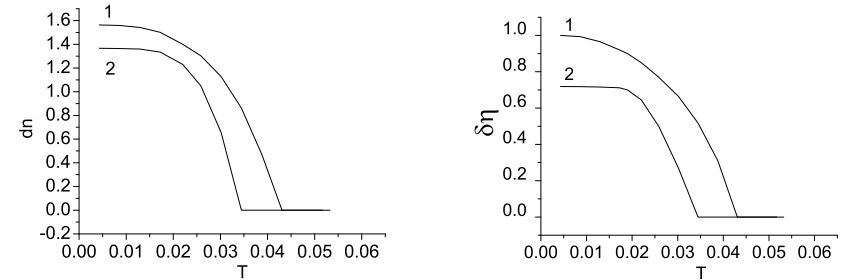
Figure 4. The temperature dependence of the values δn and $\delta \eta$ along the phase transition line, 1 - $\Omega = 0$; 2 - $\Omega = 0.05 eV$.

4. Dynamic conductance of quasi-one-dimensional structures with hydrogen bonds

Calculation of dynamic conductance of the structure which posses the chains with hydrogen bonds was carried out according to formula Kubo [21]

$$\sigma(\omega, T) = \frac{1}{Na} \int\limits_0^\infty dt \exp[i(\omega + i\varepsilon)t] \int\limits_0^\beta d\lambda \langle \hat{j}(t - i\hbar\lambda)\hat{j}(0) \rangle, \qquad (10)$$

where $\hat{j}$ is the current density operator

$$\hat{j}(0) = \frac{i}{\hbar}[\hat{H}, \hat{d}], \qquad (11)$$

$\hat{d}$ is the dipole momentum operator

$$\hat{d} = (-e) \sum_l \sum_i R_i(l) n_i(l) + z_H^{eff} \delta \sum_l \sum_i S_i^z(l),$$

that includes electronic and pseudospin (ionic) part. Here δ is a distance between equilibrium positions of a proton on the bond, $\delta \approx 0.40$ Å. According to quantum-chemical calculations the effective charge of hydrogen z_H^{eff} is equaled $z_H^{eff} \approx 0.25e$

$$j(t) = e^{\frac{i}{\hbar}Ht} j(0) e^{-\frac{i}{\hbar}Ht}. \qquad (12)$$

In approach of a molecular field the operator of current density is parted on the total electronic and proton (pseudo-spin) terms

$$\hat{j} = \hat{j}_e + \hat{j}_{sp}. \tag{13}$$

For these composite such expressions are obtained:

$$\hat{j}_e(0) = -\frac{2e}{\hbar}\sum_{k,\alpha}(\frac{\partial E_\alpha(k)}{\partial k_z} - (-1)^\alpha 2E_\alpha(k)F(k))a_{k,\alpha}^+ a_{k,\alpha} + \tag{14}$$

$$\frac{2e}{\hbar}\sum_{k}F(k)(E_1(k) - E_2(k))(a_{k,2}^+ a_{k,1} + a_{k,1}^+ a_{k,2}) \tag{15}$$

$$\hat{j}_{sp}(0) = \frac{i}{2}\frac{\delta}{\hbar}\Omega z_H^{eff}\sum_{l}\sum_{i,\alpha}(S_{i,\alpha}^-(l) - S_{i,\alpha}^+(l)). \tag{16}$$

Calculation of correlation functions in expression (10) with use of the Vick theorem yields the following expressions for an real part of conductance:

$$\sigma = \sigma_e + \sigma_{sp}, \tag{17}$$

Where the electronic part has a such form:

$$\sigma_e(\omega) = \frac{4\pi e^2}{Na\hbar^2}\beta\sum_{k,\alpha}(\frac{\partial E_\alpha(k)}{\partial k_z} - (-1)^\alpha 2E_\alpha(k)F(k))^2$$

$$\times\frac{e^{\beta(E_\alpha(k)-\mu)}}{(1+e^{\beta(E_\alpha(k)-\mu)})^2}\delta(\omega) +$$

$$\frac{4\pi e^2}{Na\hbar^2}\sum_{k}F(k)^2(E_2(k) - E_1(k))\frac{(e^{\beta(E_2(k)-\mu)} - e^{\beta(E_1(k)-\mu)})}{(1+e^{\beta(E_1(k)-\mu)})(1+e^{\beta(E_2(k)-\mu)})}$$

$$\times(\delta(\omega + \frac{1}{\hbar}(E_2(k) - E_1(k))) + \delta(\omega - \frac{1}{\hbar}(E_2(k) - E_1(k)))) \tag{18}$$

Here

$$F(k) = -\frac{1}{2}\frac{g(\eta_1 - \eta_2)t_k'}{g^2(\eta_1 - \eta_2)^2 + t_k^2}$$

For the proton part of conductance we have:

$$\sigma_{sp}(\omega) = \frac{\pi}{2a}\left(\frac{\delta}{2\hbar}z_H^{eff}\Omega\right)^2\sum_{\alpha}\frac{1}{\lambda_\alpha}\frac{1-e^{-\beta\lambda_\alpha}}{1+e^{-\beta\lambda_\alpha}}\left(\delta(\omega-\lambda_\alpha/\hbar) + \delta(\omega+\lambda_\alpha/\hbar)\right). \tag{19}$$

Frequency dependence of electronic part of the dynamical conductivity along the phase transition line is shown in Fig.5, where curve 1 denotes the state before phase transition (uniform phase), while curves 2 and 3 correspond to the state after phase transition (modulated structure). At the phase transition from uniform to modulated structure the conductance $\sigma_e(0)$, when $\omega = 0$, is abruptly reduced by two to three orders of magnitude at low temperatures and with increasing temperature decreases the value of the jump. Electronic conductance has one peak (at $\omega = 0$) in uniform phase (one electron zone is considered). We observed the splitting of the electron band in modulated phase and electronic conductivity has a broad maximum in the frequency region $\omega = \frac{1}{\hbar}(E_2(k) - E_1(k))$ as well as a peak in $\omega = 0$. This broad maximum placed in the lower frequencies for the structures with high proton tunneling frequency and stronger direct interaction between protons. The value of conductivity $\sigma_e(0)$ in modulated phase increase with temperature. The value of the dynamical conductivity $\sigma_e(\omega)$ decreases with increasing temperature and its maximum shifts to lower frequency region and vanishes at the critical temperature when there is no modulated structure. In a homogeneous phase only one peak remains at $\omega = 0$. The change of the frequency dependence of the dynamical conductivity with the parameters j and μ is shown in Fig.6 and Fig.7, here we consider $h = 0$. It is obtained that maximum of the dynamical conductivity decreases and shifts to lower frequency region with increasing the parameters j and μ. It is exist a critical values of these parameters (see Fig.1) when the modulated phase vanishes and remains only peak at $\omega = 0$. The temperature dependence of electronic conductivity $\sigma_e(0)$ is shown in Fig.8. This part of the conductivity is higher for systems with greater proton tunneling frequency in hydrogen bond and it increases with increasing the parameters j. Conductivity value is given in relative units.

Proton dynamic conductivity has peaks at frequencies corresponding protons energies λ_i on hydrogen bonds $\omega_i = \frac{\lambda_i}{\hbar}$. One peak (λ_0) for the case of homogeneous phase and two peaks (λ_1, λ_2) for case of modulated structure.

5. Conclusion

The possibility of the first- or the second-order transitions from uniform phase into phase with doubled lattice period in the quasi-one-dimensional structures with hydrogen bonds is studied in framework of proposed pseudospin-electron model. It was shown that pseudospin-electron (proton-electron) interaction may cause the appearance of charge ordered phase in the structures with hydrogen bonds. The elec-
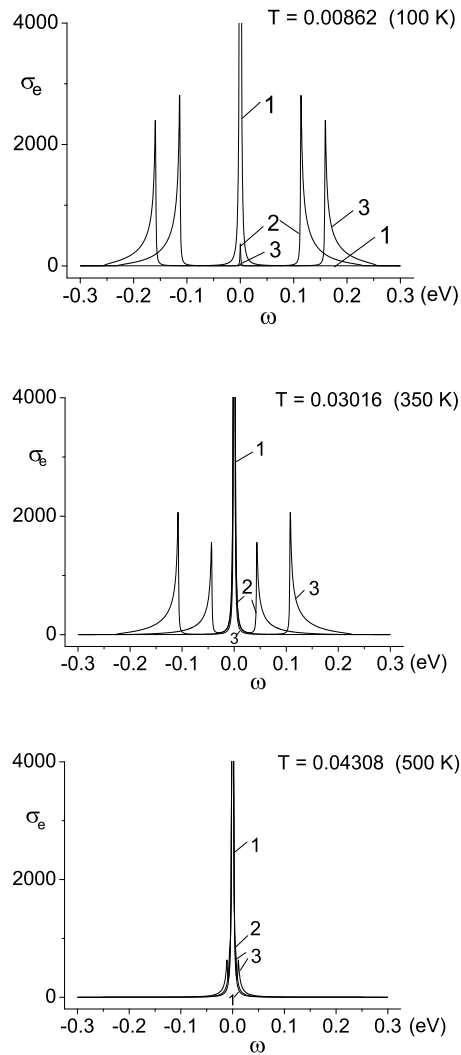
Figure 5. Frequency dependence of electronic part of conductance: 1 - before phase transition (uniform phase), $2, 3$ - after phase transition (modulated structure) along the phase transition line; 3 - $\Omega = 0$; 2 - $\Omega = 0.05 eV$, $\mu = 0$, $j = 0$.
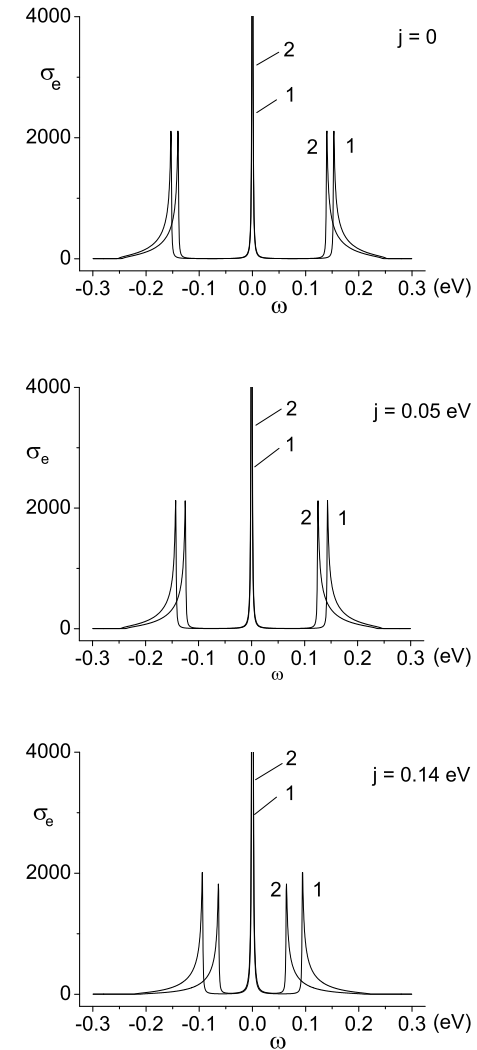

Figure 6. Frequency dependence of electronic part of conductance with different value of proton-proton interaction (parameter j), $h = 0$, $\mu = 0$, $T = 0.03016(350K)$: $j = 0; 0.05; 0.14$; 1 - $\Omega = 0$; 2 - $\Omega = 0.05 eV$.
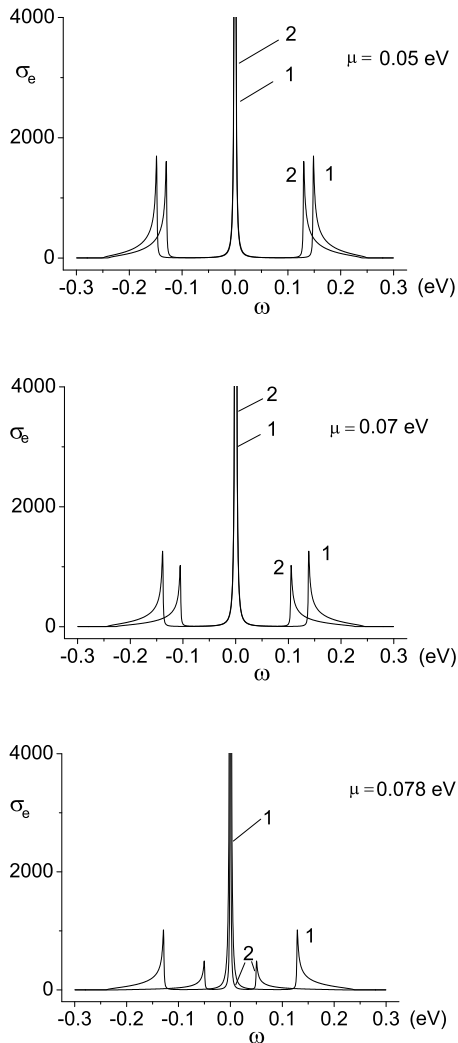
Figure 7. Frequency dependence of electronic part of conductance with different value of chemical potential μ; $h = 0$, $j = 0$, $T = 0.03016(350K)$: $\mu = 0.05; 0.07; 0.078$; 1 - $\Omega = 0$; 2 - $\Omega = 0.05eV$.
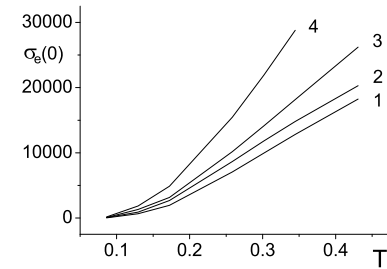

Figure 8. Temperature dependence of electronic part of conductance of the modulated structure $\sigma_e(0)$; $\mu = 0$; $1, 2$ - $j = 0$; 3 - $j = 0.05$; 4 - $j = 0.12$; 1 - $\Omega = 0$; $2, 3, 4$ - $\Omega = 0.05eV$.

tron spectrum is calculated. The dependence of the splitting of the electron spectrum on temperature and asymmetry field are investigated. The dependence of the electron concentration and mean number of protons on site on temperature and asymmetry field were obtained. It was shown, that abruptly changes of this characteristics at the first-order transitions is smaller for the structures with high proton tunneling frequency and stronger direct interaction between protons. The phase transition lines from uniform phase into charge ordered phase is determined. The dependence of the dynamical conductivity on temperature and external field and it changes at the phase transitions are obtained. At the phase transition from uniform to modulated structure the conductance $\sigma_e(0)$, when $\omega = 0$, is abruptly reduced by two to three orders of magnitude at low temperatures and with increasing temperature decreases the value of the jump. Electronic conductance has one peak at $\omega = 0$ in uniform phase. In modulated phase the dynamical electronic conductivity has a broad maximum as well as a peak in $\omega = 0$. This broad maximum placed in the lower frequencies for the structures with high proton tunneling frequency and stronger direct interaction between protons. It was shown, that frequency dependence of the proton dynamical conductivity has a one peak in uniform phase and two peaks in the charge modulated phase. The model can be applied to describe of quasi-one-dimensional structures so-called halogen-bridge mixed-valence transition-metal complexes [3] in which there are charge modulated states.

References

1. Stasyuk I.V., Stetsiv R.Ya., Sizonenko Yu.V., Condensed Matter Physics **5**, 685 (2002).
2. Stasyuk I.V., Stetsiv R.Ya., Yurechko R.Ya., J. Physical Studies, **9**, No.4, 349 (2005).
3. Okaniwa K., Okamoto H., Mitani T., Toriumi K. and Yamashita M., J. Phys. Soc. Japan **60**, No.3, 997 (1991).
4. Mitani T., Kitagawa H., Okamoto H., Nakasuji K., Toyota J., Yamashita M., Mol. Cryst. Liq. Cryst. **216**, 73 (1992).
5. N. Matsushita, K. Toriumi, N. Kojima, Mol. Cryst. Liq. Cryst. **216**, 201 (1992).
6. Y. Morimoto, Y. Tokura, T. Oohashi, T. Kojima, A. Itsubo, Mol. Cryst. Liq. Cryst., **216**, 223 (1992).
7. K. Okaniwa, H. Okamoto, T. Mitani, T. Inabe, J. Tojoda, Y.Morita, K. Nakasyji Mol. Cryst. Liq. Cryst. **216**, 241 (1992).
8. Takeda S., Chihara H., Inabe T., Mitani T. and Maruyama Y., Mol. Cryst. Liq. Cryst. **216**, 235 (1992).
9. Nakasuji K., Sugiura K., Toyoda J., Morita Y., Okamoto H., Okaniwa K., Mitani T., Mol. Cryst. Liq. Cryst. **216**, 213 (1992).
10. Inabe T., Okaniwa K., Okamoto H., Mitani T., Maruyama Y., Takeda S., Mol. Cryst. Liq. Cryst. **216**, 229 (1992).
11. Stasyuk I.V., Sizonenko Yu.V., Stetsiv R.Ya., J. Physical Studies, **2**, No.4, 463 (1998).
12. Hillenbrand E.A. and Scheiner S., J. Amer. Chem. Soc. **106**, No.21, 6266 (1984).
13. Scheiner S. Extraction of the principles of proton transfers by *ab-initio* methods. - In: Proton Transfer in Hydrogen-Bonded Systems. Edited by T. Bountis, Plenum Press, New York, 1992, pp. 29-50
14. Zhao X.G. and Cukier R.I., J. Phys. Chem., **99**, 945 (1995)
15. Cukier R.I., J. Phys. Chem., **100**, 15428 (1996)
16. Fang J.-Y. and Hammes-Schiffer S., J. Chem. Phys., **106**, 8442 (1997)
17. Fang J.-Y. and Hammes-Schiffer S., J. Chem. Phys., **107** (15), 5727 (1997)
18. Matsushita E., Phys.Rew. B, **51**, 17332 (1995)
19. Stasyuk I.V., Shvaika A.M., Tabunshchyk K.V., Condens. Matter Phys. **2**, 109 (1999); Ukr. Fiz. Zh. **45**, 520 (2000).
20. Stasyuk I.V., Mysakovych T.S., J. Physical Studies **5**, No. 3/4, 268 (2001).
21. Kubo R., J. Phys. Soc. Jpn., **12**, 570 (1957).

CONDENSED MATTER PHYSICS

The journal **Condensed Matter Physics** is founded in 1993 and published by Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine.

AIMS AND SCOPE: The journal **Condensed Matter Physics** contains research and review articles in the field of statistical mechanics and condensed matter theory. The main attention is paid to physics of solid, liquid and amorphous systems, phase equilibria and phase transitions, thermal, structural, electric, magnetic and optical properties of condensed matter. Condensed Matter Physics is published quarterly.