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ATTRACTIVE INTERACTIONS OF SPIN POLARONS IN THE QUASI-ONE-DIMENSIONAL SPIN-DENSITY-WAVE BACKGROUND

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Abstract The dynamics of spin polarons (spin bags) in the quasi-one-dimensional spin-density-wave background is numerically studied using the extended Peierls-Hubbard model. Interchain couplings are incorporated to the model as a staggered magnetic field. Time-dependent unrestricted Hartree-Fock equations and Newtonian equations are solved using Suzuki's decomposition of exponential operators. In the Hubbard model, the spin polarons with antiparallel spin polarizations attract each other. When the nearest-neighbor Coulomb repulsion is included, the interaction changes to a repulsive type. Further addition of an intersite electron-phonon coupling leads to an attractive interaction.

INTRODUCTION

Nonlinear excitations, such as solitons and polarons, in quasi-one-dimensional (1D) materials have attracted much attention.[1] The quasi-1D materials have a rich variety of ground states, depending on the strengths of electron-phonon and electron-electron interactions: bond-order-wave (BOW), charge-density-wave (CDW), spin-density-wave (SDW), spin-Peierls, and superconducting (SC) states. Static and dynamical properties of the solitons in the BOW, CDW and SDW backgrounds were extensively studied. However, only few aspects are known on the dynamics of the polarons.

In the present paper, we study the dynamics of the polarons in the SDW background, putting emphasis on interactions between two polarons with like charges and antiparallel spins. We examine the effects of the nearest-neighbor Coulomb repulsion and the electron-phonon coupling on the polaron-polaron interactions. Interchain couplings are included to the 1D extended Peierls-Hubbard model in the form of a staggered magnetic field. This quasi-1D model is of great interest because it can also be considered as an analog of two-dimensional models usually used in theoretical studies of high-T_c superconductors.[2,3]

MODEL AND METHOD FOR NUMERICAL CALCULATION

We have studied the 1D extended Peierls-Hubbard model with the staggered magnetic field:

$$\begin{aligned}\mathcal{H} = &-\sum_{i,s}[t_0 - \alpha(u_{i+1} - u_i)](\mathrm{e}^{+\mathrm{i}\gamma A_s}c^\dagger_{i,s}c_{i+1,s} + \mathrm{e}^{-\mathrm{i}\gamma A_s}c^\dagger_{i+1,s}c_{i,s}) \\ &+ U\sum_i(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) + V\sum_i(n_i - 1)(n_{i+1} - 1) \\ &- H\sum_i(-1)^i(n_{i\uparrow} - n_{i\downarrow}) + \sum_i\frac{K}{2}u_i^2 + \sum_i\frac{p_i^2}{2M}. \end{aligned} \tag{1}$$

Here $c^\dagger_{i,s}$ ($c_{i,s}$) creates (annihilates) an electron with spin s on the ith site. U and V are, respectively, the on-site and nearest-neighbor Coulomb repulsions, t_0 the hopping integral between neighboring ions in the undimerized state, α the intersite electron-phonon coupling, u_i the lattice displacement of the ith ion, H the strength of the staggered magnetic field, M the mass of an ion, K a coefficient of the lattice-distortion potential, and p_i the momentum conjugate to u_i. A_s is the vector potential giving rise to a spin-dependent electric field $E_s = -(1/c)\dot{A}_s$. The parameter γ is defined by $\gamma = ea/(\hbar c)$, where e is the absolute value of the electronic charge, a the distance between the neighboring ions in the undimerized state and c the light velocity. The hopping integral is assumed to depend linearly on the bond length between the neighboring ions. As for the lattice-distortion potential, we have assumed a purely quadratic dependence. This type of electron-phonon model corresponds to a BOW limit of the single-band model proposed by Baeriswyl and Bishop.[4]

The time-dependent unrestricted Hartree-Fock equation for single-particle electronic wave functions is written as

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial\psi_{\nu,s}(i,t)}{\partial t} = &-\left\{\mathrm{e}^{+\mathrm{i}\gamma A_s}[t_0 - \alpha(u_{i+1}(t) - u_i(t))] + V\tau_s(i,t)\right\}\psi_{\nu,s}(i+1,t) \\ &-\left\{\mathrm{e}^{-\mathrm{i}\gamma A_s}[t_0 - \alpha(u_i(t) - u_{i-1}(t))] + V\tau_s^*(i-1,t)\right\}\psi_{\nu,s}(i-1,t) \\ &+\left\{U\left[\rho_{-s}(i,t) - \frac{1}{2}\right] + V\sum_{s'}[\rho_{s'}(i+1,t) + \rho_{s'}(i-1,t) - 1]\right. \\ &\left. - (-1)^i sH\right\}\psi_{\nu,s}(i,t), \end{aligned} \tag{2}$$

with

$$\rho_s(i,t) = \sum_\nu{}'\psi^*_{\nu,s}(i,t)\psi_{\nu,s}(i,t) \quad \text{and} \quad \tau_s(i,t) = \sum_\nu{}'\psi^*_{\nu,s}(i+1,t)\psi_{\nu,s}(i,t). \tag{3}$$

Here the prime attached to the summation symbol denotes the sum over the single-particle states occupied at the initial time, s being $+1$ or -1 depending on spin-up or spin-down. The equation of motion for the lattice variables is determined by the following Newtonian equation:

$$M\ddot{u}_i = -Ku_i + \alpha\sum_s\left\{\mathrm{e}^{+\mathrm{i}\gamma A_s}[\tau_s^*(i,t) - \tau_s^*(i-1,t)] + c.c.\right\}. \tag{4}$$

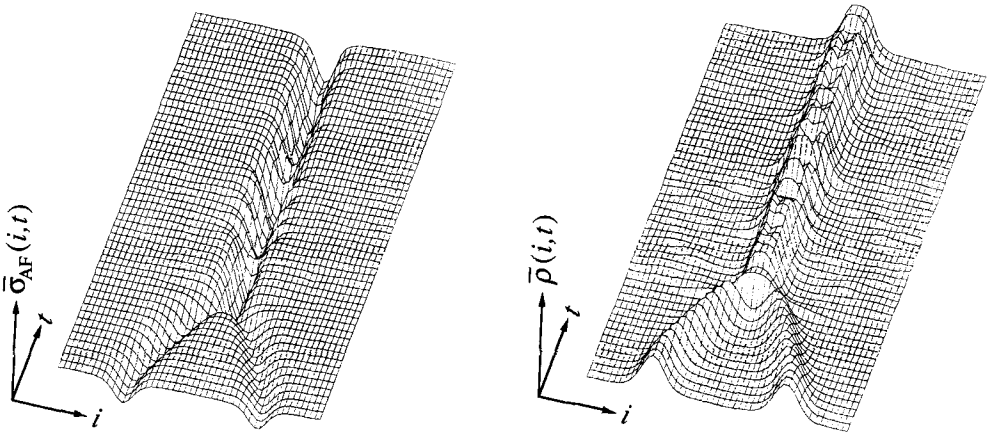

FIGURE 1 The stereographic representations of the antiferromagnetic spin density $\bar{\sigma}_{AF}(i,t)$ and the excess charge density $\bar{\rho}(i,t)$ for the case of $V=0$ and $\lambda=0$. The final time is $1000\hbar/t_0$.

The time-differential equations, (2) and (4), can be integrated with the help of Suzuki's decomposition of exponential operators.[5] Details of the numerical method for solving (2) are given in ref. 6.

RESULTS

The numerical calculations have been performed on a ring satisfying the periodic boundary condition. We have chosen the total number of lattice points $N = 98$ and the total number of electrons $N_e = 100$. As an initial state, we prepare a pair of spin polarons; one with an up-spin being located on the 25th site, and the other with a down-spin on the 74th site. Each polaron has a negative charge.

We have accelerated the polarons by applying a (fictitious) spin-dependent electric field. The time-dependence of the field has been

$$E_s(t) = \begin{cases} sE_0(1-\cos\dfrac{2\pi t}{\tau}), & \text{for } 0 \le t \le \tau, \\ 0, & \text{for } \tau < t, \end{cases} \tag{5}$$

with $s = \pm 1$. The duration τ should be longer than a typical time scale of the system, $\hbar/t_0$. The strength E_0 should be weak enough. Throughout the present paper, we use $\tau = 100\hbar/t_0$ and $E_0 = 0.00025t_0/(ea)$. For the parameters appearing in the Hamiltonian, the following values are assumed: $U = 2.5t_0$, $H = 0.01t_0$, $\hbar\omega \equiv \hbar\sqrt{K/M} = 0.1t_0$. We examine three cases for V and $\lambda \equiv \alpha^2/Kt_0$: (i) $V = 0$, $\lambda = 0$, (ii) $V = 0.75t_0$, $\lambda = 0$, and (iii) $V = 0.75t_0$, $\lambda = 0.0625$.

Figure 1 shows space and time dependences of the antiferromagnetic (AF) spin density and the excess charge density for the first case. Here the AF spin density is smoothed in the space coordinate as $\bar{\sigma}_{AF}(i,t) = (-1)^i[-\sigma(i-1,t)+2\sigma(i,t)-\sigma(i+1,t)]/4$ with $\sigma(i,t) = \sum_s s\rho_s(i,t)$. The excess charge density is also smoothed as $\bar{\rho}(i,t) = [\rho(i-1,t)+2\rho(i,t)+\rho(i+1,t)]/4-1$ with $\rho(i,t) = \sum_s \rho_s(i,t)$. It is clearly seen that

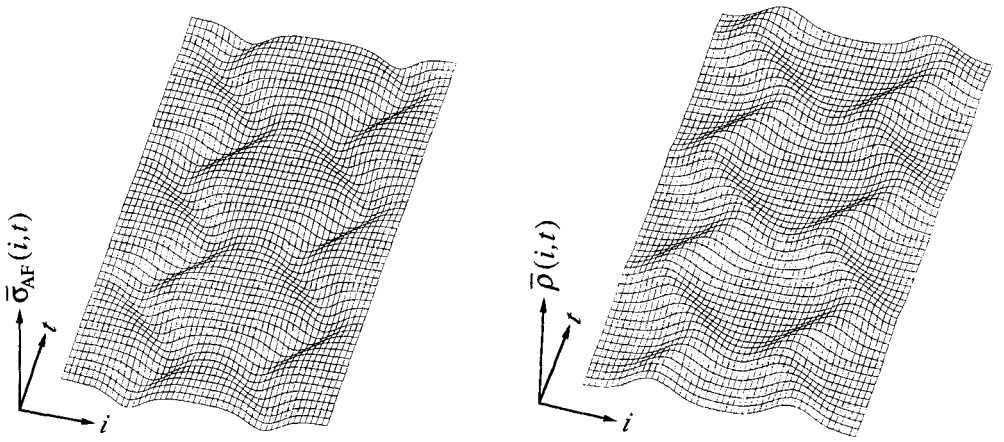

FIGURE 2 The same as Fig. 1 for the case of $V = 0.75t_0$ and $\lambda = 0$.

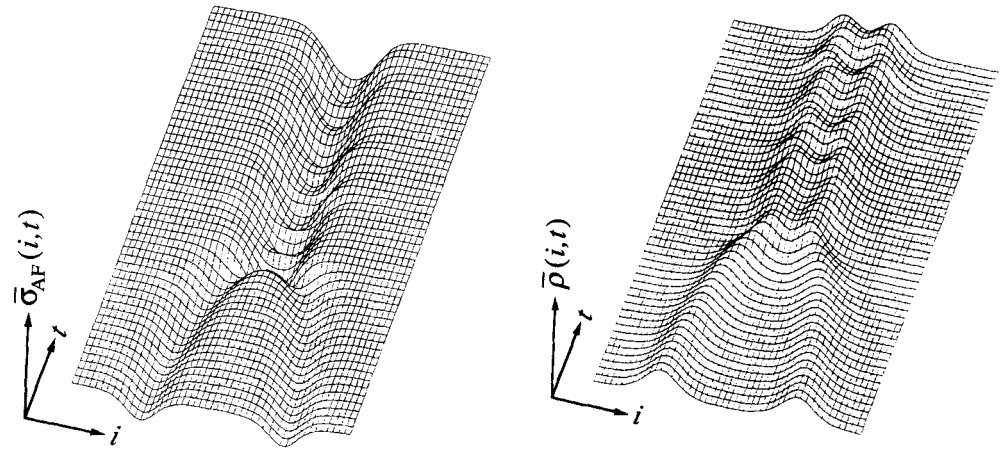

FIGURE 3 The same as Fig. 1 for the case of $V = 0.75t_0$ and $\lambda = 0.0625$.

the polarons attract each other, collide together and eventually make a bound state *bipolaron*. After the collision, the bipolaron continues to oscillate.

Figure 2 shows the AF spin density and the excess charge density for the second case. The behavior of the polarons is quite different from that of the previous case. The polarons repel each other and reflect to opposite directions. Because of the periodic boundary condition, the polarons collide again and again. At each collision, the polarons repel each other. The polaron mass is smaller compared with the first case, which fact comes from the wider extent of the polaron.

In Fig. 3, we show the AF spin density and the excess charge density for the third case. The polarons attract each other, being trapped to form a bipolaron state. Again an oscillation is observed after the collision. It should be noted that the polarons are weakly bound compared with the first case. The polaron has larger mass than that of the first case because of dressing phonons around itself.

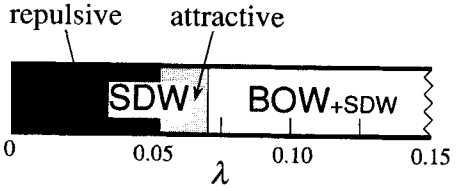

FIGURE 4 (above) The phase diagram of the Hartree-Fock ground state in the half-filled case, along with the interaction between the polarons. Parameters are $U = 2.5t_0$, $V = 0.75t_0$ and $H = 0.01t_0$.

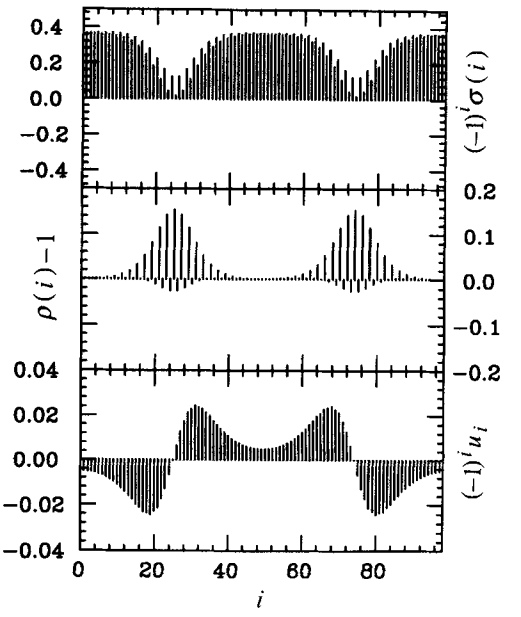

FIGURE 5 (right) The staggered spin density $(-1)^i\sigma(i)$, the excess charge density $\rho(i) - 1$ and the staggered lattice displacement $(-1)^i u_i$ for the polaron pair at the initial state.

Fixing the nearest-neighbor repulsion at $V = 0.75t_0$, we have studied a few cases with different values of λ. The results are sketched in Fig. 4. For the half-filling, the SDW state is energetically most favorable for $\lambda \lesssim 0.07$. At $\lambda \sim 0.07$, there is a first-order phase transition from the SDW state to the BOW state mixed with small amplitude of the SDW order. In the neighborhood of the phase boundary, there is a small region where the interaction between the polarons is attractive.

DISCUSSION

In the present paper, we have studied the dynamics of a pair of polarons with like charges and antiparallel spin polarizations. The one-dimensional extended Peierls-Hubbard model with a staggered magnetic field is studied within the framework of the time-dependent unrestricted Hartree-Fock approximation. When only the on-site Coulomb repulsion is taken into account, the polarons attract each other, being trapped to form a bipolaron state. This polaron binding is analogous to the formation of bipolarons in the electron-phonon model with a non-degenerate ground state.[7,8] This is consistent with calculations in the two-dimensional Hubbard model treated within the Hartree-Fock[9] and spin-fluctuation[10,11] theories. This is also consistent with exact-diagonalization studies[2] of small clusters, as well as Hartree-Fock studies[3] of large systems, in the one-dimensional Hubbard (and t-J) model with the staggered magnetic field. When the nearest-neighbor repulsion is included to the Hubbard model, the polarons repel each other. Further addition of the intersite electron-phonon coupling changes the interaction to an attractive type again.

The polaron-polaron interaction can be understood in the following way. Figure 5 shows the staggered spin density, the excess charge density and the staggered

lattice displacement of the polaron pair at the initial state. Each polaron has a local depression of the staggered spin density. The polaron sitting on the 25th site has excess charge density mainly at odd-numbered sites, while the other polaron on the 74th site at even-numbered sites. When the polarons approach each other, this charge distribution does not change; the left (right) polaron has excess charge density mainly on odd(even)-numbered sites. Thus the matrix element of the on-site Coulomb repulsion is very small due to the vanishingly small overlap between the excess charge densities of the polarons. Therefore, in the Hubbard model, the polarons attract each other by sharing a common region of the depression of the staggered spin density. On the other hand, the matrix element of the nearest-neighbor Coulomb repulsion becomes large when the polarons come close to each other. This repulsive force overcomes the attractive force above a critical value of V_c ($V_c < 0.75t_0$ in the present case). As for the role of the electron-phonon coupling, the polarons enhance the lattice displacement cooperatively when approaching each other. This enhancement reduces the electronic energy, making it possible for the polarons to attract each other. We should note here that this pairing mechanism has some relevance to the recently proposed SC pairing mechanism in dimerized and undimerized t-J models.[12]

Before concluding the present paper, we should make some remarks. In the present paper, we have used the time-dependent Hartree-Fock approximation. We cannot exclude the possibility of the quantum tunneling of the polarons even in the presence of the nearest-neighbor Coulomb repulsion. In order to go beyond the mean-field type approximation, we are now studying small clusters by exact-diagonalization method. The results will be reported in the future. In the present paper, we have considered the intersite electron-phonon coupling. The effects of the site-diagonal coupling are also of great significance and will be studied in the future.

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