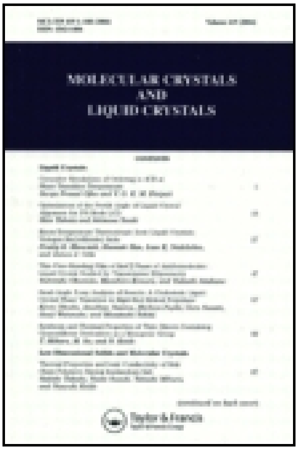

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SPIN GAP IN ONE-DIMENSIONAL ELECTRON-PHONON SYSTEMS

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Abstract The exponents of spin and charge correlations of one-dimensional electron systems are calculated by a renormalization-group method. We study combined effects of electron-phonon interaction and the Umklapp process on renormalization flows. As scattering processes are successively integrated out, these two processes are interfered with each other depending on the type of electron-phonon coupling, phonon frequency and filling. We demonstrate how these factors control a spin gap formation and density-wave/superconductor correlations.

INTRODUCTION

One-dimensional materials have rich phase diagrams due to the instability of the Fermi liquid against any of electron-phonon and electron-electron interactions. The instability is strong at half filling due to the commensurability or the Umklapp process so that most of them are insulators. If the filling can be controlled, doping of charge carriers may cause them to be metallic. Nevertheless electron correlations are generally important near half filling since the Umklapp process is effective at a doping-dependent finite-energy range. For electron-phonon systems without electron correlations, nearly-half-filled states are well described by charged or neutral solitons[1] in the background of a charge density wave or a bond order wave. Combined effects of electron-phonon and electron-electron interactions[2] are much less known due to technical difficulties. They are essential to understand metal-insulator transitions in organic-inorganic hybrid, π-d systems[3] since they have both π-characters and d-characters. A renormalization-group method is convenient in one dimension where scaling properties are well known for purely electron systems.[4] It can be extended to electron-phonon systems[5] and is used here to investigate the combined effects near half filling. The details of the derivation of equations were reported elsewhere.[6]

MODEL

We consider continuum models in which the electronic dispersion relation around the Fermi points is linearized with velocities $\pm v_F$ so that electron fields are bosonized. We take on-site electron repulsion of strength U for which all the scattering parameters, $g_{1\parallel}$, $g_{1\perp}$, g_2, g_3 and g_4,[4] are initially equal to U in the lowest order. It is known that the spin and charge degrees of freedom are separated in the asymptotic limit: the spin part is characterized by the parameter K_σ defined by $K_\sigma^2 = (2\pi v_F - g_4 + g_{1\parallel})/(2\pi v_F - g_4 - g_{1\parallel})$ and the backscattering $g_{1\perp}$, while the charge part by the parameter K_ρ defined by $K_\rho^2 = (2\pi v_F + g_4 + g_{1\parallel} - 2g_2)/(2\pi v_F + g_4 - g_{1\parallel} + 2g_2)$ and the Umklapp process g_3. Without $g_{1\perp}$ and g_3, the charge-density-wave, spin-density-wave, singlet-superconductor, and triplet-superconductor correlations are known to be proportional to $r^{-K_\sigma - K_\rho}$, $r^{-K_\sigma^{-1} - K_\rho}$, $r^{-K_\sigma - K_\rho^{-1}}$, and $r^{-K_\sigma^{-1} - K_\rho^{-1}}$, respectively, in the Euclidean space. The interactions $g_{1\perp}$ and g_3 modify K_σ and K_ρ into K_σ^* and K_ρ^*, respectively, where the asterisk denotes a fixed-point value of the renormalization-group equation below. $K_\nu^* = 0$ corresponds in the present order to the Luther-Emery state[7] which has a gap in the ν excitation spectrum. We define dimensionless parameters by $X_\sigma = 2(1 - K_\sigma^{-1}) \simeq g_{1\parallel}/(\pi v_F)$, $Y_\sigma = g_{1\perp}/(\pi v_F)$, $X_\rho = 2(1 - K_\rho^{-1}) \simeq (g_{1\parallel} - 2g_2)/(\pi v_F)$, and $Y_\rho = g_3/(\pi v_F)$. A filling factor $\delta n = n - 1$ is so defined that $\delta n = 0$ corresponds to the half filling. A cutoff α is used in the boson representation, which is of the order of the inverse Fermi wave number. Then $2\pi \delta n \alpha$ is dimensionless.

As to electron-phonon interaction, we consider the continuum limits of the Holstein coupling,[8]

$$\sum_i \left(\beta q_i n_i + \frac{K}{2} q_i^2 + \frac{1}{2M} p_i^2 \right) , \tag{1}$$

with electron density at site i, n_i, lattice displacement q_i, its conjugate momentum p_i, coupling strength β, spring constant K, and ionic mass M, and of the Su-Schrieffer-Heeger (SSH) coupling,[1]

$$\sum_i \left[\alpha_s (q_{i+1} - q_i) \sum_s (c_{i,s}^\dagger c_{i+1,s} + c_{i+1,s}^\dagger c_{i,s}) + \frac{K}{2} (q_{i+1} - q_i)^2 + \frac{1}{2M} p_i^2 \right] , \tag{2}$$

with $c_{i,s}$ annihilating an electron with spin s at site i, α_s being the coupling strength, and q_i, p_i, K and M as above. The former coupling causes back and forward scatterings of dimensionless strengths $Y_1 = \beta^2/(\pi v_F K)$ and $Y_2 = \beta^2/(\pi v_F K)$, respectively, while the latter coupling causes a backward scattering of strength $Y_1 = 4\alpha_s^2/(\pi v_F K)$. The backward scatterings have different form factors, which are distinguished here by $f = 1$ in the former and $f = -1$ in the latter. The difference is evident in the antiadiabatic limit ($\omega/E_{\rm F} \to \infty$, where ω is the phonon frequency and $E_{\rm F}$ is the Fermi energy): the Holstein coupling is reduced to the attractive Hubbard coupling $-(\beta^2/K)\sum_i c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow}$ corresponding to backward scattering parameters $g_{1\parallel} = g_{1\perp} = g_3 = -\beta^2/K$ and forward scattering parameters $g_2 = g_4 = -\beta^2/K$, while the SSH coupling to $-(\alpha_s^2/2K)\sum_{i,s,s'}(c^\dagger_{i,s}c_{i+1,s} + c^\dagger_{i+1,s}c_{i,s})(c^\dagger_{i,s'}c_{i+1,s'} + c^\dagger_{i+1,s'}c_{i,s'})$ corresponding to $g_{1\parallel} = g_{1\perp} = -g_3 = -4\alpha_s^2/K$ and $g_2 = g_4 = 0$. Note the sign of g_3. Thus the electron-phonon interaction simply shifts the parameters by $X_\sigma \to X_\sigma - Y_1$, $Y_\sigma \to Y_\sigma - Y_1$, $X_\rho \to X_\rho - (Y_1 - 2Y_2)$, and $Y_\rho \to Y_\rho - fY_1$ in this limit.

To study the differences coming from the form factors, we use the continuum limit of the Holstein-Hubbard model ($f = 1$) and that of the SSH-Hubbard model supplemented with a forward scattering Y_2 ($f = -1$) both with $X_\sigma = Y_\sigma = -X_\rho = Y_\rho \equiv Y_{\rm el} = U/(\pi v_{\rm F}) > 0$ and $Y_1 = Y_2 \equiv Y_{\rm ph}$.

RENORMALIZATION FLOWS

Renormalization-group equations are derived before.[6] As the energy scale is made smaller with increasing l as $E(l) = E_{\rm F}e^{-l}$, the effective values of X_σ, Y_σ, X_ρ, Y_ρ, $2\pi\delta n\alpha$, Y_1, and Y_2 vary according to

$$dX_\sigma(l)/dl = -Y_\sigma^2(l) - Y_1(l)D(l)\,, \tag{3}$$

$$dY_\sigma(l)/dl = -X_\sigma(l)Y_\sigma(l) - Y_1(l)D(l)\,, \tag{4}$$

$$dX_\rho(l)/dl = -Y_\rho^2(l)J_0(2\pi\delta n(l)\alpha) - [Y_1(l) - 2Y_2(l)]D(l)\,, \tag{5}$$

$$dY_\rho(l)/dl = -X_\rho(l)Y_\rho(l) - fY_1(l)D(l)\,, \tag{6}$$

$$d(2\pi\delta n(l)\alpha)/dl = 2\pi\delta n(l)\alpha + Y_\rho^2(l)J_1(2\pi\delta n(l)\alpha)\,, \tag{7}$$

$$dY_1(l)/dl = [2 - K_\sigma(l) - K_\rho(l) - Y_\sigma(l) - fY_\rho(l)J_0(2\pi\delta n(l)\alpha)]Y_1(l)\,, \tag{8}$$

$$dY_2(l)/dl = 0\,. \tag{9}$$

We cut off the Bessel functions $J_n(x)$ at $j_{0,1}$ by $J_n(x)\theta(j_{0,1} - |x|)$, where $j_{0,1}$ is the first zero of $J_0(x)$. $D(l) = [\omega/E(l)]\exp[-\omega/E(l)]$ is a phonon propagator. Initial conditions are: $X_\sigma(0) = X_\sigma - Y_1h(\omega/E_{\rm F})$, $Y_\sigma(0) = Y_\sigma - Y_1h(\omega/E_{\rm F})$, $X_\rho(0) = X_\rho - (Y_1 - 2Y_2)h(\omega/E_{\rm F})$, and $Y_\rho(0) = Y_\rho - fY_1h(\omega/E_{\rm F})$, with $h(x) = 1 - e^{-x}$, which correctly reproduce the $\omega = \infty$ limit.

Without electron-phonon coupling, $Y_1(l)$ or $Y_2(l)$, the fixed-point values are well known and easily obtained: $X_\sigma^* = 0$ and $K_\sigma^* = 1$ so that the spin excitation spectrum is gapless; at half filling, $X_\rho^* = -\infty$ and $K_\rho^* = 0$ so that a charge gap opens; otherwise, the Umklapp process, $Y_\rho(l)$, is cut off by $J_0(2\pi\delta n(l)\alpha)$ so that the charge excitation spectrum is gapless and the system is metallic with a finite Drude weight. With $Y_1(l)$ included, coupling of spin and charge occurs and it becomes a maximum at $E(l) \simeq \omega$ due to $D(l)$. For $E(l) \ll \omega$ $[D(l) \ll 1]$, the retarded couplings $Y_1(l)$ and $Y_2(l)$ have been absorbed into the effective electronic parameters. Deviation from half filling, $2\pi\delta n(l)\alpha$, grows with decreasing energy scale, i.e., with increasing length scale, corresponding to the increasing number of charged solitons inside the length α. The filling dependence occurs through $Y_\rho^{(2)}(l)J_0(2\pi\delta n(l)\alpha)$: the cut-off energy for Y_ρ is zero (i.e., no cut off) at half filling and increases with $| \delta n |$. Through $Y_1(l)$, the spin correlation also depends on the filling.

The differences coming from the sign of f are demonstrated in the evolution of renormalized quantities. The phonon-assisted backward scattering $Y_1(l)$ is interfered with the Umklapp process $Y_\rho(l)$ destructively for $f = 1$ (FIG. 1) and constructively for $f = -1$ (FIG. 2). It is reflected on the value of $Y_1(l)D(l)$ relative to that of $Y_2(l)D(l)$: it is smaller for $f = 1$ and larger for $f = -1$. Note that the Umklapp process $Y_\rho(l)$ is cut off at a much higher energy ($l \simeq 2$) than ω ($l \simeq 5$). It is found (not shown here) that, as ω decreases, the interference becomes more effective, so that the filling dependence of K_ρ^* is larger. The evolution of $X_\rho(l)$ here is mainly due to $Y_\rho(l)$ for $l \lesssim 2$ and due to $Y_1(l)$ and $Y_2(l)$ for $l \gtrsim 2$. In both cases, $X_\rho^* < 0$ and $K_\rho^* < 1$ so that the density-wave correlation is dominant over the superconductor correlation. In order for the latter to be dominant ($X_\rho^* > 0$ and $K_\rho^* > 1$), $Y_\rho(l)$ and $Y_1(l)$ have to be small enough. Therefore, larger deviation from half filling and the destructive interference ($f = 1$) are favorable to the superconductor correlation. Generally, the phonon-mediated superconductor phase has a spin gap, but the spin gap does not necessarily mean a dominant superconductor correlation. The fixed point of the spin correlation exponent, K_σ^*, is determined by the sign of $X(l)$ after the $Y_1(l)$ term is integrated out: $K_\sigma^* = 1$ if it is positive and $K_\sigma^* = 0$ (a spin gap) if it is negative. With the parameter set used here and $f = 1$, the destructively interfered $Y_1(l)$ does not grow large enough to open a spin gap (FIG. 1). Meanwhile, with $f = -1$, $Y_1(l)$ grows large enough to make $X_\sigma(l)$ negative (FIG. 2): $K_\sigma^* = 0$ and a spin gap opens.

In summary, $Y_1(l)$ grows larger for $f = -1$, smaller $2\pi\delta n\alpha$, and smaller ω due to the interference with $Y_\rho(l)$. These conditions are favorable to a spin gap. Meanwhile, $Y_1(l)$ and $Y_\rho(l)$ act against the superconductor correlation. Consequently, upon doping, a metallic phase with a spin gap and a dominant charge-density-wave correlation generally appears before a superconductor phase with a spin gap. For $Y_2 = 0$, the superconductor phase disappears, but the metallic spin-gap phase survives, which

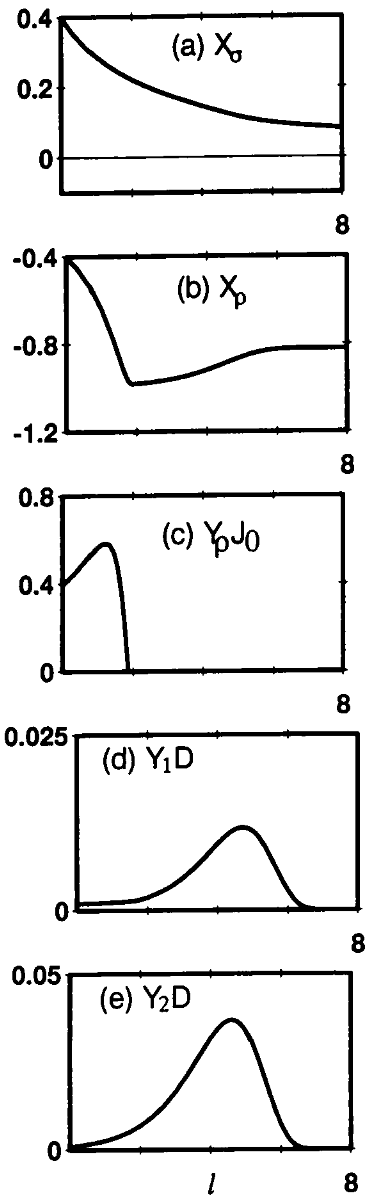

FIGURE 1 (a) X_σ, (b) X_ρ, (c) $Y_\rho J_0(2\pi\delta n\alpha)$, (d) $Y_1 D$, and (e) $Y_2 D$, as functions of l, of the Holstein-Hubbard model. Initial parameters are $Y_{el} = 0.4$, $2\pi\delta n\alpha = 0.25$, $Y_{ph} = 0.1$, and $\omega/E_F = 0.01$.

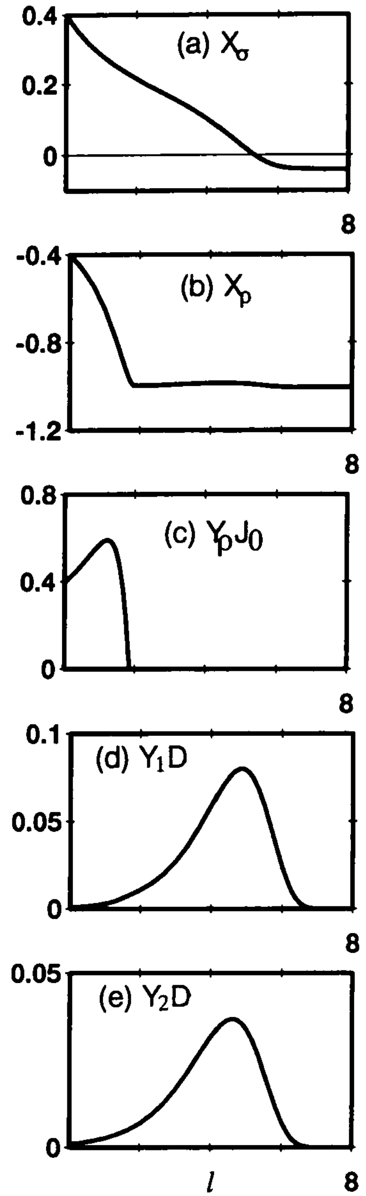

FIGURE 2 (a) X_σ, (b) X_ρ, (c) $Y_\rho J_0(2\pi\delta n\alpha)$, (d) $Y_1 D$, and (e) $Y_2 D$, as functions of l, of the SSH-Hubbard model supplemented with Y_2. Initial parameters are $Y_{el} = 0.4$, $2\pi\delta n\alpha = 0.25$, $Y_{ph} = 0.1$, and $\omega/E_F = 0.01$.

would be realized when a spin-Peierls system is doped.

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