Fluctuation Effects by Boson Dispersion in Fermion-boson Coupled Systems

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Abstract. Nonlinear feedback effects due to dispersive bosons are studied in fermion-boson coupled systems by using an extension of dynamical mean-field theory. In the nonperturbative regime, strong coupling and nonadiabaticity reduce effective interaction between fermions as the width of boson dispersion increases. The boson field is completely softened at the crossover to this regime. The softening is significantly enhanced by the boson dispersion. We elucidate the controlling parameters of this nonperturbative regime where fluctuations of the dispersive bosons accelerate the delocalization of fermions.

INTRODUCTION

Control of bandwidth or dispersion of fermions relative to the interaction strength has been the subject of a great deal of theoretical and experimental works. Tuning of the fermion dispersion has been extensively studied, for instance, in terms of localization-delocalization problems such as the Mott transition [1]. Compared with this situation, effects of boson dispersion have been paid less attention in this field. Bosons have been considered in the limit of zero dispersion (Einstein bosons) in many studies of fermion-boson coupled systems [2, 3].

Dispersion of bosons is, however, relevant in many realistic systems. For instance, phonon modes in various oxide materials are dispersive due to intersite coupling through oxygens shared by adjacent unit cells. This should be relevant to variety of cooperative phenomena of lattice and charge degrees of freedom in those materials.

In this contribution, we study dispersive bosons interacting with fermions using dynamical mean-field (DMF) theory. The DMF theory provides a local view of a many-body problem in terms of an impurity problem obeying a self-consistency condition [4]. The DMF method is extended to include feedback effects through the fermion-boson interaction [5]. We control the width of the boson dispersion to examine fluctuation effects of boson fields.

FORMALISM AND MODEL

For the fermion-boson coupled systems, the action for a local view by the DMF theory has the general form [4, 5]

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$$S_{\mathrm{eff}} = \int d\tau d\tau' [\sum_{\alpha} c_{\alpha}^{\dagger}(\tau) g_{0\alpha}^{-1}(\tau-\tau') c_{\alpha}(\tau') + \sum_{\nu} x_{\nu}(\tau) D_{0\nu}^{-1}(\tau-\tau') x_{\nu}(\tau')]$$
$$+ \int d\tau \sum_{\alpha_1\alpha_2\nu} \lambda_{\alpha_1\alpha_2\nu} c_{\alpha_1}^{\dagger}(\tau) c_{\alpha_2}(\tau) x_{\nu}(\tau), \tag{1}$$

where g_0 and D_0 are the Weiss fields for fermion and boson, respectively. Note that the action (1) is quite general which contains also fermion interactions such as the Coulomb repulsion through the Hubbard-Stratonovich transformation [6, 7].

The full Green's functions g and D are related to the Weiss fields by $g_{\alpha}^{-1}(i\omega_n) = g_{0\alpha}^{-1}(i\omega_n) - \Sigma_{\alpha}(i\omega_n)$ and $D_{\nu}^{-1}(i\omega_n) = D_{0\nu}^{-1}(i\omega_n) - \Pi_{\nu}(i\omega_n)$, where Σ and Π are the self-energy for fermion and boson, respectively. The DMF framework is extended to determine both g and D simultaneously by the self-consistency conditions

$$g_{\alpha} = \sum_{\mathrm{q}} [i\omega_n + \mu - \varepsilon_{\mathrm{q}_{\alpha}} - \Sigma_{\alpha}]^{-1}, \quad D_{\nu} = \sum_{\mathrm{q}} [(i\omega_n)^2 - \omega_{\mathrm{q}_{\nu}}^2 - \Pi_{\nu}]^{-1} \tag{2}$$

where $\varepsilon_{\mathrm{q}_{\alpha}}$ and $\omega_{\mathrm{q}_{\nu}}$ give the dispersion relations for fermions and bosons, respectively. Here the bosons are described as harmonic oscillators.

In the following sections, the above DMF equations are examined for a simple model with fermions interacting with one branch of bosons, which is a straightforward extension of the so-called Holstein model [3] to include the boson dispersion:

$$H = \sum_{\alpha=1,2} \sum_{ij} t_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + \frac{M}{2} (\sum_{i} \dot{x}_i^2 + \sum_{ij} \omega_{ij}^2 x_i x_j) + \lambda \sum_{\alpha,i} (c_{i\alpha}^{\dagger} c_{i\alpha} - \frac{1}{2}) x_i. \tag{3}$$

We focus on the half-filled case in the DMF solutions without any symmetry breaking at low temperatures.

The DMF theory has been tested to give useful insights into three-dimensional systems [4]. We therefore assume semicircular density of states for both fermions and bosons as $D_F(\varepsilon) = 2\sqrt{W^2 - \varepsilon^2} / \pi W^2$ and $D_B(\varepsilon) = 2\sqrt{\omega_1^2 - (\varepsilon - \omega_0)^2} / \pi \omega_1^2$ where W is the half-bandwidth of the fermion density of states; ω_0 and ω_1 are the center and the half-bandwidth of the boson density of states, respectively.

The action (1) is solved by quantum Monte Carlo method. Details of the method and conditions of calculations are reported elsewhere [5].

RESULTS

In this section, effects of the boson dispersion are examined in the boson Weiss field D_0 and the imaginary part of the fermion self-energy ImΣ. Both quantities are closely connected with the effective interaction between fermions. In particular, D_0 is directly related to the retarded effective interaction between fermions as $U_{\mathrm{eff}} = \lambda^2 D_0$ when the bosons are integrated out. We take three independent paramaters, ω_0, $U \equiv U_{\mathrm{eff}}(\omega_1 = 0) = \lambda^2 / \mathrm{M}\omega_0^2$, and ω_1 in the energy unit $W = 1$.

In the perturbative regimes, i.e., in the weak-coupling limit ($W \gg \omega_0$, U) and in the atomic limit ($W \ll \omega_0$, U), both $|D_0|$ and $|\mathrm{Im}\Sigma|$ increase as ω_1 increases in our DMF solutions. This indicates that the effective interaction between fermions is enhanced by the width of the boson dispersion. The results are consistent with the perturbative arguments [8, 3, 2].

In contrast to this, both $|D_0|$ and $|\mathrm{Im}\Sigma|$ decrease as ω_1 increases in the nonperturbative regime, i.e., in the strong coupling region away from the anti-adiabatic limit ($U > W$ and $\omega_0 \sim W$). Surprisingly, the effective interaction between fermions are weakened by the dispersive bosons.

Fig. 1(a) shows the boson Weiss field $|D_0|$ as a function of ω_1 for various values of U. The fermion self-energy $|\mathrm{Im}\Sigma|$ changes in a similar way. For small U, $|D_0|$ increases by ω_1, as in the perturbative regime. When the value of U increases, a kink appears and $|D_0|$ decreases for larger values of ω_1. This kink corresponds to the crossover from the perturbative to the nonperturbative regime.

The crossover is correlated well with the complete softening of the boson field. Fig. 1(b) exhibits the effective frequency of the boson field defined by a pole of the boson Green's function as $\omega^* = \sqrt{(\omega_0 - \omega_1)^2 + \Pi(i\omega_n = 0)}$, where Π is the self-energy for boson. ω^* goes to zero at the value of ω_1 where $|D_0|$ shows a kink. The nonperturbative regime is characterized by the weakening of the effective interaction due to the strong boson fluctuations and by the softening of the boson field.

DISCUSSIONS

A systematic study of the crossover for various ω_0 and U elucidates two important parameters in the present system [5,9]. One is the pair formation energy divided by the fermion kinetic energy u, and the other is the fermion-boson coupling divided by

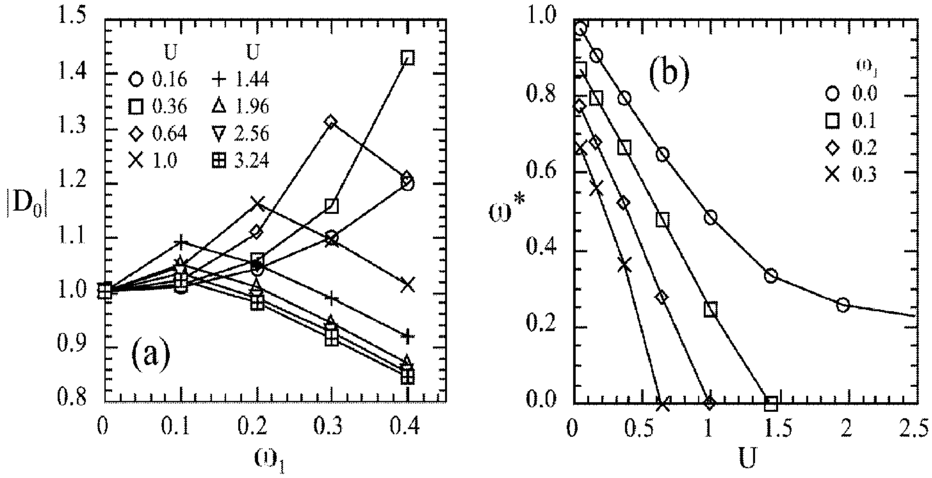

FIGURE 1. DMF solutions for $\omega_0 = 1$ at the inverse temperature $\beta = 8$; (a) the boson Weiss field at zero Matsubara frequency and (b) the effective frequency of the boson field.

the stored energy in the boson field η. The former describes the competition between the itinerant character and the localization of fermions. The latter distinguishes the single-boson and the multiboson regimes. The both conditions $u > 1$ and $\eta > 1$ are necessary to cause the crossover accompanied by the complete softening of bosons.

Our DMF solutions in the regime with $u > 1$ and $\eta > 1$ indicate a reduction of the effective interaction by the boson dispersion. Strong boson fluctuations tend to accelerate the delocalization of fermions and to make polarons unstable. This striking result is revealed for the first time by our extended DMF method which successfully includes the mutual feedback in many-body systems. Note that the criteria of $u > 1$ and $\eta > 1$ have been discussed for the formation of a small polaron in a system with a single fermion interacting with bosons [10, 11]. In the single-fermion problem, however, there is no feedback to bosons from changes of the fermion state in the thermodynamic limit.

The softening of the boson field is significantly affected by the boson dispersion. Small width of the dispersion reduces the crossover value of U markedly. The reduction is notable especially for $\omega_0 > W$. For instance, in the case of $\omega_0 = 4$, the boson field is completely softened at $U = 4$ when $\omega_1 = 0.2$ ($\omega_1 / \omega_0 = 5\%$) although ω^* remains finite even at $U = 16$ for the dispersionless case. This is a consequence of the strongly nonlinear feedbacks by dispersive bosons.

The softening may be related with charge freezing accompanied by a lattice ordering in electron-phonon problems if we allow symmetry breakings in an unfrustrated model. Therefore, our results strongly suggest the importance of the boson dispersion in describing cooperative phenomena of lattice and charge degrees of freedom. More realistic models are under investigation which include orbital degrees of freedom of electrons, several modes of phonons, and Coulomb interactions.

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