Interplay of electron–phonon interaction and strong correlations: DMFT+Σ approach

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ABSTRACT

We discuss interaction of strongly correlated electrons (described within the Hubbard model solved by dynamical mean-field theory (DMFT)) with Debye and Einstein phonons using recently developed DMFT+Σ computational scheme. Electron–phonon interaction (EPI) is analyzed in adiabatic approximation (assuming the validity of Migdal theorem), allowing the neglect of EPI vertex corrections. This approach is valid for EPI coupling constant $\lambda < \varepsilon_F/\omega_{ph} \sim 10$, where ε_F is Fermi energy and ω_{ph} is Debye or Einstein frequency. For moderate values of λ only small changes in the electronic density of states are observed in DMFT+Σ approximation for both weakly and strongly correlated metallic regimes. Metal–insulator (Mott) transition due to the increase of Hubbard interaction U is slightly inhibited by EPI. Our main aim is to discuss the interplay of "kinks" in electronic dispersion due to EPI and recently discovered kinks of electronic origin. For the certain region of model parameters coexistence of phonon "kinks" in electronic dispersion with purely electronic "kinks" is readily observed and we formulate some simple criteria of such coexistence. However, for most general combinations of model parameters phonon "kinks" make electronic "kinks" hardly observable. In the general case an increase of Hubbard interaction U rapidly suppresses the slope of electronic dispersion within the phonon "kink." These results are important for deeper understanding of the shape and evolution of electronic dispersions in strongly correlated systems such as copper oxides, where different kinds of "kinks" were recently observed in ARPES experiments.

1. Introduction

The problem of the interplay of strong electronic correlations with electron–phonon interaction is of central importance in the physics of highly correlated systems. Actually there is rather long history of such studies, e.g. one of the most popular models for electron–phonon interaction (EPI) in strongly correlated systems is the so-called Hubbard–Holstein model (HHM). The Hubbard model [1] itself describes local Coulomb interaction of electrons on a lattice including e.g. Mott–Hubbard metal–insulator transition. On the other hand Holstein model contains local linear displacement-to-density interaction of conducting electrons with local (Einstein) phonon modes [2].

Active investigations of the properties of the HHM were undertaken in the framework of dynamical mean-field theory (DMFT) [3], which is a non-perturbative approach with respect to interaction parameters of the Hubbard model. Among many others one should mention DMFT solution of HHM for the case where impurity solver used was the numerical renormalization group (NRG) [4]. The mapping of HHM to Anderson–Holstein impurity was first performed by Hewson and Mayer [5]. It was shown that using NRG one can compute in a numerically exact manner total electron–phonon contribution to the self-energy of the problem, thus making solution of the HHM non-perturbative also with respect to electron–phonon coupling strength.

However, up to now there are apparently no studies of strongly correlated electrons interacting with Debye phonons. It is even more surprising in view of the widely discussed physics of kinks in electronic dispersion observed in ARPES experiments 40–70 meV below the Fermi level of high-temperature superconductors [6], which are often attributed to EPI [7]. To our knowledge problem of kink formation on electronic dispersion caused by EPI in strongly correlated systems was briefly discussed within HHM in papers by Hague [9] and Koller et al. [8].

In this paper we consider the influence of Debye or Einstein phonons on the weakly and strongly correlated electrons within our recently developed DMFT+Σ approach, studying electron dispersion and density of states (DOS), in particular close to Mott–Hubbard metal–insulator transition. We analyze in details how EPI affects electronic dispersions in correlated metal and discuss the interplay of recently discovered kinks of purely electronic nature in electronic dispersion [10] and usual phonon kinks in the electronic spectra.

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2. DMFT+Σ computational details

The major assumption of our DMFT+Σ approach is that the lattice and time Fourier transform of the single-particle Green function can be written as

$$G_{\mathbf{p}}(\varepsilon) = \frac{1}{\varepsilon + \mu - \varepsilon(\mathbf{p}) - \Sigma(\varepsilon) - \Sigma_{\mathbf{p}}(\varepsilon)} \quad (1)$$

where $\varepsilon(\mathbf{p})$ is the bare electron dispersion, $\Sigma(\varepsilon)$ is the *local* self-energy of DMFT, while $\Sigma_{\mathbf{p}}(\varepsilon)$ is some "external" (in general case momentum dependent) self-energy. Advantage of our generalized approach is the additive form of the self-energy (neglect of interference) in Eq. (1) [11–13]. It allows one to keep the set of self-consistent equations of standard DMFT [3]. However, there are two distinctions. First, on each DMFT iterations we recalculate corresponding "external" self-energy $\Sigma_{\mathbf{p}}(\mu,\varepsilon,[\Sigma(\varepsilon)])$ within some (approximate) scheme, taking into account interactions e.g. with collective modes (phonons, magnons etc.) or some order parameter fluctuations. Second, the local Green's function of effective impurity problem is defined as

$$G_{ii}(\varepsilon) = \frac{1}{N}\sum_{\mathbf{p}} \frac{1}{\varepsilon + \mu - \varepsilon(\mathbf{p}) - \Sigma(\varepsilon) - \Sigma_{\mathbf{p}}(\varepsilon)}, \quad (2)$$

at each step of the standard DMFT procedure.

Eventually, we get the desired Green function in the form of (1), where $\Sigma(\varepsilon)$ and $\Sigma_{\mathbf{p}}(\varepsilon)$ are those appearing at the end of our iteration procedure.

To treat electron–phonon interaction for strongly correlated system we just introduce $\Sigma_{\mathbf{p}}(\varepsilon) = \Sigma_{ph}(\varepsilon,\mathbf{p})$ due to electron–phonon interaction within the usual Fröhlich model. To solve single impurity Anderson problem we use NRG [4]. All calculations are done at nearly zero temperature and at half filling. For "bare" electrons we assume semielliptic DOS with half-bandwidth D.

According to the Migdal theorem in adiabatic approximation [14] we can restrict ourselves with the simplest first order contribution to $\Sigma_{ph}(\varepsilon,\mathbf{p})$, neglecting vertex corrections due electron–phonon coupling which are small over adiabatic parameter $(\omega_D,\omega_0)/\varepsilon_F \ll 1$ [14]:

$$\Sigma_{ph}(\varepsilon,\mathbf{p}) = ig^2 \sum_{\omega,\mathbf{k}} \frac{\omega_0^2(\mathbf{k})}{\omega^2 - \omega_0^2(\mathbf{k}) + i\delta}$$
$$\times \frac{1}{\varepsilon + \omega + \mu - \varepsilon(\mathbf{p}+\mathbf{k}) - \Sigma(\varepsilon+\omega) - \Sigma_{ph}(\varepsilon+\omega,\mathbf{p}+\mathbf{k})} \quad (3)$$

where g is the usual electron–phonon interaction constant, $\omega_0(\mathbf{k})$ is phonon dispersion, which in our case is taken as in the standard Debye or Einstein model

$$\omega_0(\mathbf{k}) = \begin{cases} uk, & k < \dfrac{\omega_D}{u} \\ \omega_0, & k < k_0 \end{cases}. \quad (4)$$

Here u is the sound velocity, ω_D and ω_0 are Debye and Einstein frequencies with cut-off k_0 of the order of Fermi momentum p_F.

Actually $\Sigma_{ph}(\varepsilon,\mathbf{p})$ defined by Eq. (3) has weak momentum dependence which we can omit and continue only with significant frequency dependence. For Debye spectrum of phonons Eq. (3) can be rewritten as (cf. similar analysis in Ref. [18])

$$\Sigma_{ph}(\varepsilon) = \frac{-ig^2}{4\omega_c^2} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left\{ \omega_D^2 + \omega^2 \ln\left|\frac{\omega_D^2 - \omega^2}{\omega^2}\right| \right.$$
$$\left. + i\pi\omega^2 \theta(\omega_D^2 - \omega^2) \right\} I(\varepsilon+\omega) \quad (5)$$

with a characteristic frequency $\omega_c = p_F u$ of the order of ω_D, while for Einstein spectrum:

$$\Sigma_{ph}(\varepsilon) = \frac{ig^2 k_0^2}{16\pi p_F^2} \left\{ -i\pi(I(\varepsilon+\omega_0) + I(\varepsilon-\omega_0)) + \int_0^\infty \frac{d\omega}{\omega}(I(\varepsilon+\omega_0+\omega) \right.$$
$$\left. + I(\varepsilon-\omega_0-\omega) - I(\varepsilon+\omega_0-\omega) - I(\varepsilon-\omega_0+\omega)) \right\} \quad (6)$$

with

$$I(\varepsilon) = \int_{-D}^{+D} d\xi \frac{N_0(\xi)}{E_\varepsilon - \xi}. \quad (7)$$

where $E_\varepsilon = \varepsilon - \Sigma(\varepsilon) - \Sigma_{ph}(\varepsilon)$. For the case of semielliptic non-interacting DOS $N_0(\varepsilon)$ with half-bandwidth D we get

$$I(\varepsilon) = \frac{2}{D^2}(E_\varepsilon - \sqrt{E_\varepsilon^2 - D^2}), \quad (8)$$

It is convenient to introduce the dimensionless electron–phonon coupling constant as [18]

$$\lambda_D = g^2 N_0(\varepsilon_F)\frac{\omega_D^2}{4\omega_c^2}, \quad \lambda_E = g^2 N_0(\varepsilon_F)\frac{k_0^2}{4p_F^2}. \quad (9)$$

To simplify our analysis we shall not perform fully self-consistent calculations neglecting phonon renormalization due to EPI [18], assuming that the phonon spectrum (4) is fixed by the experiment.

3. Results and discussion

Let us start from comparison between pure DMFT and DMFT+Σ_{ph} DOSes for strong ($U/2D = 1.25$) and weak ($U/2D = 0.625$) Hubbard interaction presented in Fig. 1 on upper and low panels correspondingly. Dimensionless EPI constant (9) used in these calculations was $\lambda_D = \lambda_E = 0.8$, while Debye and Einstein frequencies were taken to be $\omega_D = \omega_0 = 0.125D$. In both cases we observe some spectral weight redistribution due to EPI. For $U/2D = 1.25$ (upper panel of Fig. 1) we see the well-developed three peak structure typical for strongly correlated metals. In the energy interval $\pm \omega_D,\omega_0$ around the Fermi energy (which is taken as zero energy at all figures below) there is almost no difference in the DOS quasiparticle peak line shape obtained from pure DMFT and DMFT+Σ_{ph}. However, outside this interval DMFT+Σ_{ph} quasiparticle peak becomes significantly broader with spectral weight coming from Hubbard bands and it is more pronounced for the case of Einstein phonons. This broadening of DMFT+Σ_{ph} quasiparticle peak leads as we show below to inhibiting of metal to insulator transition. In the case of $U/2D = 0.625$ there are no clear Hubbard bands formed but only some "side wings" are observed. Spectral weight redistribution on the lower panel of Fig. 1 is not dramatic, though qualitatively different from the case of $U/2D = 1.25$. Namely, main deviations between pure DMFT and DMFT+Σ_{ph} happen in the interval $\pm \omega_D$, where one can observe kind of "cap" in DMFT+Σ_{ph} DOS. Corresponding spectral weight goes to the energies around $\pm U$, where Hubbard bands are supposed to form. The lineshape of the "cap" is slightly different for the Debye and Einstein phonons due to different behaviors of Σ_{ph} (Eqs. (5) and (7))at energies $\pm \omega_D,\omega_0$. For Einstein phonons ImΣ_{ph} at these energies sharply drops down to zero. This leads to sharp cusps of DOS at $\pm \omega_0$ as shown at the insert in Fig. 1.

In Fig. 2 we compare the behavior of pure DMFT and DMFT+Σ_{ph} DOSes for different $U/2D$ values close to Mott–Hubbard metal–insulator transition for the case of Debye phonon spectrum. For $U/2D = 1.56$ both standard DMFT and DMFT+Σ_{ph} produce insulating solution. However, there is some difference between these solutions. The DMFT+Σ_{ph} Hubbard bands are lower and broader than DMFT ones because of additional interaction (EPI) included. With decrease of U for $U/2D = 1.51$ and 1.47 we observe that DMFT+Σ_{ph} results correspond to metallic state (with narrow quasiparticle peak at the Fermi level), while conventional DMFT still produces insulating solution. Only around $U/2D = 1.43$ both DMFT and DMFT+Σ_{ph} results turn out to be metallic. Overall DOSes lineshape is the same as discussed above. These results show that with the increase of U finite EPI slightly inhibits Mott–Hubbard
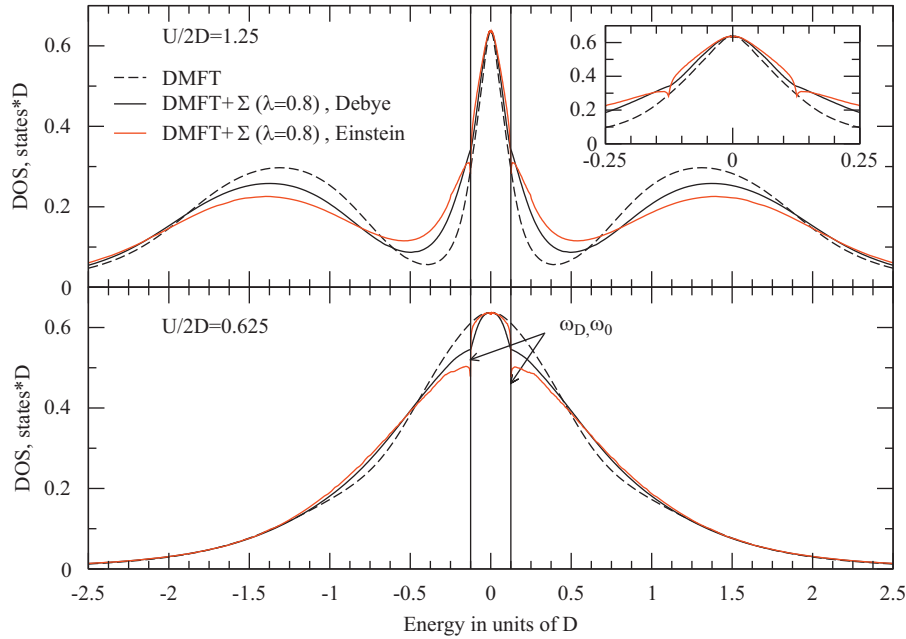
Fig. 1. Comparison of DOSes obtained within standard DMFT (dashed lines) and DMFT $+\Sigma_{ph}$ methods (solid lines) for Debye (black) and Einstein (red) phonons for strong (upper panel, $U/2D = 1.25$) and weak (lower panel, $U/2D = 0.625$) Hubbard interaction regimes. Dimensionless electron–phonon coupling constant $\lambda_D = \lambda_E = 0.8$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
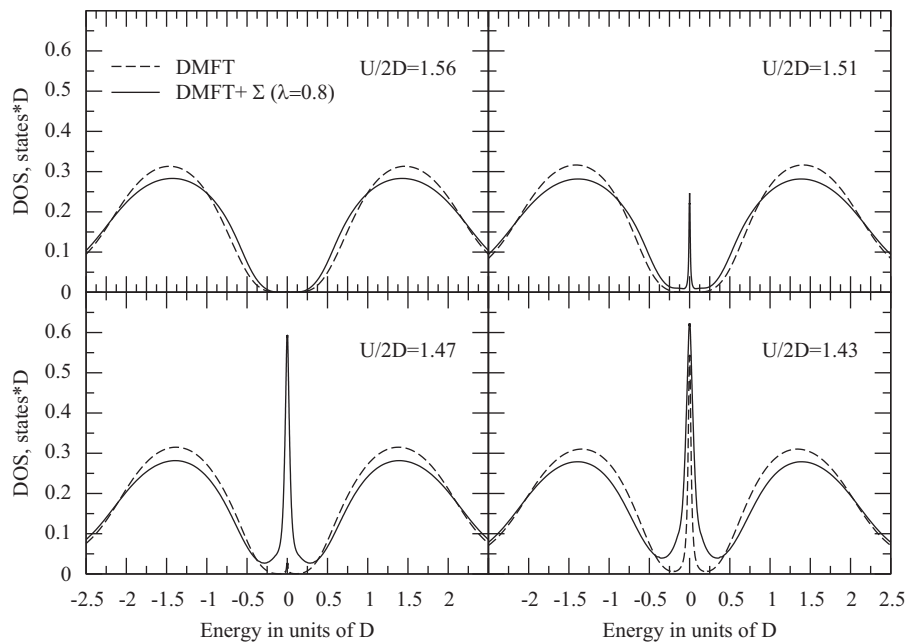

Fig. 2. Sequence of DOSes obtained within standard DMFT (dashed lines) and DMFT $+\Sigma_{ph}$ for Debye model (solid lines) methods close to metal–insulator transition (from top-left to bottom right) with $\lambda_D = 0.8$.

transition from metallic to insulating phase. For the case of Einstein phonons the MIT is inhibited even stronger. This result is similar to what was observed for the HHM in weak EPI regime [17,16,15]. For more deep insight into these results on DOS we have also analyzed the fine structure of corresponding self-energies $\Sigma(\varepsilon)$ and $\Sigma_{ph}(\varepsilon)$. Relevant details can be found in Ref. [19].

Now we address the issue of a sudden change of the slope of electronic dispersion, the so-called kinks. It is well-known that interaction of electrons with some bosonic mode always produces such a kink. In the case of EPI typical kink energy is just the Debye ω_D or Einstein ω_0 frequency. Kinks of purely electronic nature were

recently reported in Ref. [10]. The energy of purely electronic kink as derived in Ref. [10] for semielliptic bare DOS is given by

$$\omega^* = Z_{FL}(\sqrt{2}-1)D, \tag{10}$$

where D is the half of the bare bandwidth of electrons and $Z_{FL} = (1-\partial Re\Sigma)/\partial\varepsilon|_{\varepsilon = \varepsilon_F})^{-1}$ is Fermi liquid quasiparticle weight. The rough estimate of ω^* is given by the half-width of quasiparticle peak of DOS at its half-height.

Our calculations clearly demonstrate that electronic kinks are hardly observable on the background of phonon kinks and special care should be taken to separate them by rather fine tuning of the
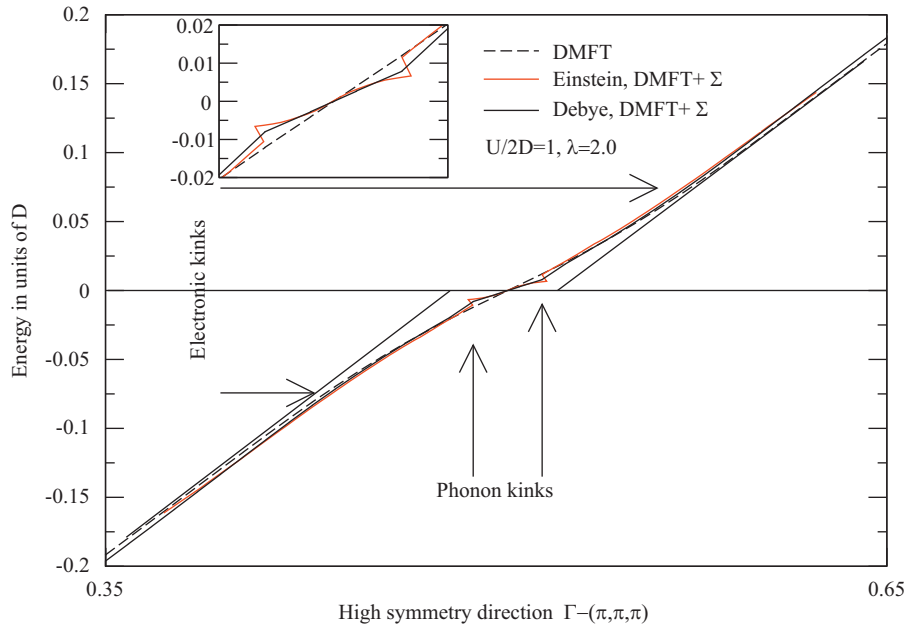
Fig. 3. Quasiparticle dispersions obtained from standard DMFT (black dashed line) and DMFT+Σ_{ph} for Debye (solid black line) and Einstein (solid red line) phonons along the part of high symmetry direction $\Gamma-(\pi,\pi,\pi)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

parameters of our model. To clarify this situation we introduce an additional characteristic of the kink—the shift of electron dispersion in momentum space δp at kink energy. From simple geometry we estimate for phonon kinks

$$\delta p_{ph} = \frac{(\omega_D, \omega_0)}{v_F} \lambda_{D,E} \qquad (11)$$

where v_F is the bare Fermi velocity and $\lambda_{D,E}$ was defined in Eq. (9). For electronic kink the similar estimate is

$$\delta p_e = \frac{\omega^*}{v_F^*} \left(1 - \frac{Z_{FL}}{Z_0}\right) \equiv \frac{\omega^*}{v_F^*} \lambda_e, \qquad (12)$$

where Z_0 is quasiparticle weight in the case of absence of electronic kinks (the same as Z_{cp} defined in Ref. [10]). Velocity v_F^* is the Fermi velocity of initial dispersion, but it cannot be just a bare one. As was reported in Ref. [10] electronic kinks can be observed only for rather strong Hubbard interaction when three peak structure in the DOS is well-developed and electronic dispersion is strongly renormalized by correlation effects. This renormalization is determined by λ_e defined in Eq. (11), which can be seen as kind of dimensionless interaction constant. In the case when both slopes on the Fermi level and out of $\pm\omega^*$ energy interval are equal there will be no electronic kink at all.

Now we can choose parameters of our model to make both kinks simultaneously visible. First of all one should take care that $\omega_D \ll \omega^*$. For $U/2D=1$ with $U = 3.5$ eV we get $\omega^* \sim 0.1D$ and a reasonable value of Debye (or Einstein) frequency is ω_D(orω_0) $\sim 0.01D$. To make phonon kink pronounced at such relatively low Debye (or Einstein) frequency (cf. Eq. (11)) we have to increase EPI constant and we take $\lambda_D = \lambda_E = 2.0$. To demonstrate coexistence of both these types of kinks we plot the energy dispersion of simple cubic lattice with nearest neighbors transfers only, along the high symmetry direction $\Gamma-(\pi,\pi,\pi)$ [10]. In Fig. 3 we show dispersion along this direction close to the Fermi level. The difference of lineshapes of Debye and Einstein kinks is illustrated at the insert in Fig. 3. As discussed above "Einstein" kink is more sharp.

Finally we address to the behavior of phonon kinks in electronic spectrum as function of Hubbard interaction U. As $U/2D$ ratio grows Fermi velocity in Eq. (11) goes down, so that momentum
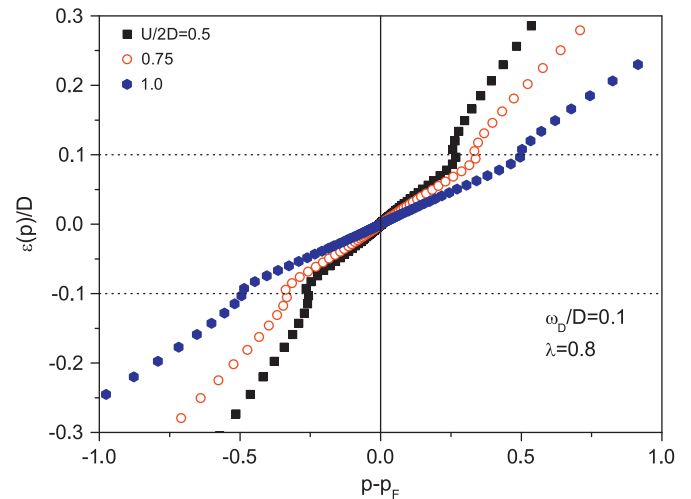

Fig. 4. Quasiparticle dispersions around Fermi level with Debye phonon kinks obtained from DMFT+Σ_{ph} calculations for different interaction strengths $U/2D = 0.5, 0.75, 1.0$; $\lambda_D = 0.8$, $\omega_D = 0.1D$.

shift of kink position δp moves away from p_F, while kink energy remains at ω_D. This is confirmed by our direct DMFT+Σ_{ph} calculations producing the overall picture of spectrum evolution shown in Fig. 4.

4. Conclusion

This work is a first attempt to analyze strongly correlated electrons, treated within DMFT approach to the Hubbard model, interacting with either Debye or Einstein phonons. EPI was treated within the simplest (Migdal theorem) approach in adiabatic approximation, allowing the neglect of vertex corrections. DMFT+Σ_{ph} approach allows us to use the standard momentum space representation for phonon self-energy (3), while the general structure of DMFT equations remains intact.

Mild EPI leads to rather insignificant changes of electron density of states, both in correlated metal and in Mott-insulator state, slightly inhibiting metal to insulator transition with increase of U. However, kinks in the electronic dispersion due to EPI dominate for the most typical values of the model parameters, making kinks of purely electronic nature, predicted in Ref. [10], hardly observable. Special care (fine tuning) of model parameters is needed to separate these anomalies in electronic dispersion in strongly correlated systems. We have also studied phonon kinks evolution with the strength of electronic correlations demonstrating the significant drop in the slope of electronic dispersion close to the Fermi level with the growth of Hubbard interaction U. Quantitative difference of results for the cases of Debye and Einstein phonon spectra was observed both in DOS and kink behavior in electronic dispersion.

Acknowledgments

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