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Charge fluctuations and electron–phonon interaction in the finite-U Hubbard model

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Abstract

Recent experiments have triggered a renewed interest for a theoretical understanding of the electron–phonon (el–ph) properties in strongly correlated systems. We employ a gaussian expansion within the finite-U slave-bosons formalism to investigate the momentum structure of the el–ph vertex function in the Hubbard model as function of U and n. The suppression of large momentum scattering and the onset of a small-$\mathbf{q}$ peak structure, parametrized by a cut-off q_c, are shown to be essentially ruled by the band narrowing factor Z_{MF} due to the electronic correlation. A phase diagram of Z_{MF} and q_c in the whole U-n space is presented. Our results are in more than qualitative agreement with a recent numerical analysis and permits the understanding of some anomalous features of the quantum Monte Carlo data.

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Keywords: Metal–insulator transition; Charge fluctuations

Recent ARPES, neutron scattering and isotope effects experiments have caused a renewed interest in the past months about electron–phonon (el–ph) effects in the high-T_c superconducting materials [1–3]. The interplay between lattice and electronic correlated degrees of freedom has been a widely debated issue. On one hand, the electronic correlation is expected to reduce the quasi-particle spectral weight Z by transferring spectral weight to quasi-localized states at high energies. On the other hand, this scenario is reflected in a strong modulation of the el–ph matrix element renormalized by the electronic correlation, with a net predominance of forward scattering at small $\mathbf{q}$ momenta [4]. So far, this important feature was analyzed only by means of analytical approaches in the $U=\infty$ limit [4,5] and a definitive confirmation of it based on numerical methods was lacking. With these motivations, in a recent paper, Huang

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et al. [6] have addressed this issue in the two-dimensional Hubbard model with generic U by using quantum Monte Carlo (QMC) techniques on a 8×8 cluster. Their results provide a good agreement with the previous analytical studies and represent an important contribution to assess the relevance of el–ph interaction in correlated systems.

In this contribution, we review some of our recent investigations [7] on this issue in the Hubbard model for generic repulsion U and generic electron filling n. To this aim, we employ a slave-boson approach which was first introduced by Kotliar and Ruckenstein [8]. In such a context, the original Hubbard Hamiltonian H is replaced by an effective one in an enlarged Hilbert space by introducing four slave-boson operators plus three Lagrange multipliers which enforce the Hilbert space within the physical one. The mean-field approximation, with respect to these auxiliary bosons and the Lagrange multipliers, describes thus a coherent band of effective non-interacting fermions with reduced spectral weight Z and reduced bandwidth $W \to ZW$. The effective scattering between electron and charge fluctuations (phonons) in the presence of strong correlation can be evaluated by expanding the slave-boson Hamiltonian beyond the mean-field solution to explicitly take into account at the leading order the electron–slave-boson scattering and the Gaussian-slave-boson fluctuations. In order to avoid unphysical divergences of the linear scattering terms between electrons and slave-bosons in the low-density limit $n \to 0$, we found subtle modifications were needed to be applied to the original scheme of Refs. [8,9].

In Fig. 1a we show the isolines for the spectral weight Z in the $U{-}\delta$ space ($\delta = 1 - n$) for a tight-binding nearest-neighbor model. U_c represents the well-known critical value of the Brinkmann–Rice transition as found by the mean-field solution. The effective el–ph matrix element $\gamma(\mathbf{q})$ and the effective el–ph coupling $\Gamma(\mathbf{q}) = |\gamma(\mathbf{q})|^2/Z$ [4] can be also evaluated as function of the exchanged momentum $\mathbf{q}$ for generic U and n. The onset of a strong predominance of forward $\mathbf{q} = 0$ scattering was found to be a generic feature as the system approaches the metal–insulator transition (MIT).

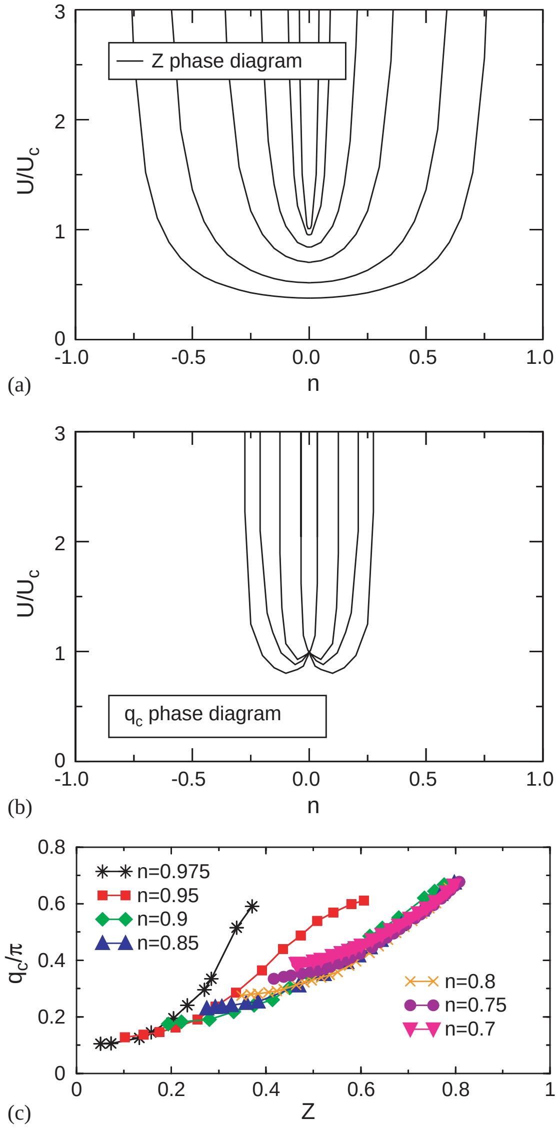

Fig. 1. Spectral weight Z isolines and Q_c isolines in the $U{-}\delta$ phase space. Solid lines correspond to (from center to the border): (a) $Z = 0.1, 0.2, 0.4, 0.6, 0.8$ 0.9; (b) $q_c/\pi = 0.1, 0.2, 0.3, 0.4$. (c) Plot of q_c vs. Z_{MF} for different electron filling n. The cutoff q_c, evaluated for different U and n, is shown to lie on an almost universal curve when plotted as a function of Z_{MF}.

A momentum cut-off q_c was defined by the full-width half-maximum criterion for the quantity $\Gamma(\mathbf{q})$. Values of q_c in the $U{-}\delta$ phase diagram are shown in Fig. 1b. The striking similarities between panels (a) and (b) in Fig. 1 points out that the small momentum selection of the el–ph coupling is essentially driven by the reduction of the spectral weight Z approaching the MIT. This is pointed out in the most remarkable way in panel (c) where the cut-off q_c, evaluated for different n and different U, is shown to lie on an almost universal curve when plotted as function of Z (small discrepancies for $n \simeq 1$ are due to the presence of the Van Hove singularity at half-filling for the nearest-neighbor tight-binding model here considered). This is quite an important result because the band narrowing factor Z, as well as quasi-particle spectral weight Z_{QP} which is strongly related to Z, is in principle a physical quantity which can be experimentally determined to provide an estimate of q_c. A comparison between our analytical approach [7] and QMC results [6] suggests in addition that the upturn of the el–ph matrix scattering for small $\mathbf{q}$ as function of the Hubbard repulsion is likely related to some tendency towards a phase separation or a charge-density-wave instability. It should be noted that the small momentum selection parametrized by q_c plays a fundamental role in the context of the nonadiabatic theory of superconductivity which could in a natural way account for high-T_c superconductivity in an unconventional el–ph framework [10].

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