Renormalization of the electron-phonon interaction in presence of charge fluctuations

R. Citro, S. Cojocaru,* and M. Marinaro
Dipartimento di Fisica "E. R. Caianiello" and Laboratorio Regionale "SuperMat," I.N.F.M. di Salerno, Università degli Studi di Salerno, Via S. Allende, I-84081 Baronissi (Sa), Italy

(Received 16 February 2005; published 12 September 2005)

We investigate the effect of strong electron correlations on the coupling of electrons to Holstein phonons in the one-band Hubbard model in the presence of charge fluctuations. Specifically, we analyze the momentum modulation of the electron-phonon vertex induced by the electronic correlations. The role of the on-site Coulomb interaction U is investigated in different regions of the Brillouin zone. The results reveal the presence of a strong forward scattering peak at low temperatures and, after an initial decrease with U, we find that the electron-phonon vertex starts to increase above an intermediate value of the Coulomb interaction. We show that this behavior is related to an incipient phase separation that takes place at a critical value of U for fixed doping. A comparison with other approaches is also discussed.

DOI: 10.1103/PhysRevB.72.115108 PACS number(s): 71.10.Fd, 71.27.+a, 71.45.Lr

The relevance of the electron-phonon (el-ph) interaction in the physics of high-T_c cuprate superconductors has recently attracted great interest. A variety of experiments display pronounced phonon and electron-lattice effects in these materials. For example, the strong renormalization of electrons near the Fermi surface at characteristic energy scales,[1] or the large isotope effect by oxygen substitution away from optimal doping observed in angle-resolved photoemission (ARPES) experiments,[1–3] give evidence of a significant el-ph coupling. These findings, accompanied by the fact that the undoped cuprates are Mott antiferromagnetic insulators whose essential physics is well described by Hubbard and t-J models, require additional understanding of the el-ph properties in strongly correlated systems. The effects of the strong electronic correlation on the el-ph properties in the one- and three-band Hubbard models have been investigated by analytical techniques based on $(1/N)$ expansion within slave bosons[4,5] and the Hubbard X-operators[6] formalisms. One finding[6] is that for the ionic el-ph coupling in the underdoped regime, the forward scattering with small phonon momentum transfer is enhanced much more than the backward scattering with large phonon momentum transfer. On the other side, the presence of a peaked forward scattering favors an attractive interaction in the $d_{x^2-y^2}$ channel.[6,7] A limitation of the above treatments was that they were carried out for infinite U. Recently, the issue of the effect of the strong electron correlations on the el-ph interaction has been addressed in the two-dimensional Hubbard model at finite U by using quantum Monte Carlo (QMC) technique on a 8×8 cluster[8] and the slave-bosons treatments based on four auxiliary fields,[9] as well as the Kotliar-Ruckenstein (KR) slave-bosons representation.[10] The QMC study reveals that entering the strong coupling regime the forward scattering begins to increase as a function of U, leading to an effective el-ph coupling which is peaked in the forward direction. On the other hand, the results of the slave-boson analysis show that the on-site Coulomb interaction U strongly suppresses the coupling to the Holstein phonon at low temperatures. Going to larger temperatures $kT\sim t$ (where t is the band width) it is found that after an initial decrease with U, the el-ph coupling starts to increase with U, in agreement with the QMC analysis. Here, we would like to gain further insight into the influence of electron correlations on the el-ph coupling for range of values of U from intermediate to strong coupling. In particular, we would like to make clearer the role of charge excitations on the puzzling features shown by the el-ph vertex at small phonon momentum. In our paper the el-ph vertex is calculated as a linear response to an external field coupled to the correlated electrons in presence of charge fluctuations. The screening of the el-ph vertex is due to the instability of a charge vertex function that describes the response of the electron-charge density. Technical details on the calculation of the charge vertex function can be found in Ref. 11, where we computed it by using a strong-coupling approach based on the cumulant expansion.[12–14]

We consider a system of interacting electrons described by the one-band Hubbard model on a square lattice with nearest-neighbor hopping t_{ij} and next-nearest-neighbor hopping t'_{ij},

$$H=\sum_{\langle i,j\rangle,\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}-\sum_{\langle\langle i,j\rangle\rangle,\sigma} t'_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}-\mu\sum_{\sigma} n_{i\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\sigma}(c_{i\sigma})$ is an electron creation (annihilation) operator with spin σ at site i, μ is the chemical potential, U is the local Coulomb interaction. For this model we want to study the influence of the electron correlations on the coupling of the electrons to an external phonon field B_i. The bare coupling to this field has the form

$$H_{\text{el-ph}}=\sum_{i,\sigma} n_{i,\sigma}B_i, \tag{2}$$

where $n_{i,\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$, $B_i=g^0u_i$, u_i is the atomic displacement and g^0 is the local el-ph coupling. Since g^0 is a constant, we set it equal to 1. The linear response of the one-particle Green's function due to the external phonon field is given by

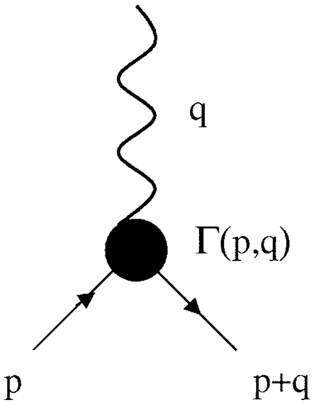

FIG. 1. Diagrammatic representation of $G_2(p,q)$. The wavy line represents the external perturbation, the straight line is the one-particle Green's function of the Hubbard model.

$$G_2(p,q) = G_1(p)\Gamma(p,q)G_1(p+q), \tag{3}$$

where $\Gamma(p,q)$ is the el-ph vertex and p and q stand for both the momentum and the Matsubara frequencies $(\mathbf{p}, i\omega_n)$ and $(\mathbf{q}, i\omega_n')$, respectively, G_1 is the single particle Green's function. Diagrammatically $G_2(p,q)$ has the structure shown in Fig. 1. Both G_2 and G_1 are evaluated with respect to the pure Hubbard Hamiltonian in Eq. (1). Since we are interested in the strong-coupling regime $(U/t \gg 1)$ they are calculated by means of the cumulant expansion to the lowest orders.[12–14]

In a recent work[15] we have shown that taking into account charge fluctuations is important to reproduce some features of quasiparticle properties observed in the high-temperature superconductors. In presence of charge fluctuations, the dressing of the electrons with charge excitations is described in terms of the scattering processes of the electron by the fluctuation. When such scattering processes are taken into account the electron-phonon vertex $\Gamma(p,q)$, depicted in Fig. 2, is given by

$$\Gamma(p,q) = \beta^{-1}\sum_{k'} G_1(k'+q)G_1(k')\Gamma^c(p-k')t_{\mathbf{k}'+\mathbf{q}}t_{\mathbf{k}'}, \tag{4}$$

where $\Gamma^c(p)$ is the charge vertex function describing the charge fluctuation and $t_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ is the hopping term, in which we are expanding. In the lowest order cumulant expansion[16] the one-particle Green's function has the following expression:

$$G_1(p) = \sum_{i=1,2} \frac{A_i(\mathbf{p})}{i\omega_n - \epsilon_{i\mathbf{p}}}, \tag{5}$$

where

$$A_1(\mathbf{k}) = \frac{\varepsilon_{1\mathbf{k}} - U(1 - \langle n_{-\sigma}\rangle)}{\varepsilon_{1\mathbf{k}} - \varepsilon_{2\mathbf{k}}} = 1 - A_2(\mathbf{k}), \tag{6}$$

while $\epsilon_{1,2\mathbf{k}} = \frac{1}{2}[U \mp t_{\mathbf{k}} - \sqrt{(U+t_{\mathbf{k}})^2 - 4t_{\mathbf{k}}(1-\langle n_{-\sigma}\rangle)U}] - \mu$, is the energy dispersion of the two Hubbard subbands, μ being the chemical potential, $\langle n_{-\sigma}\rangle$ is the average number of electrons with spin $-\sigma$. Since we are interested in the scattering processes with charge fluctuations near the Fermi surface only the contribution from the lowest subband is relevant.

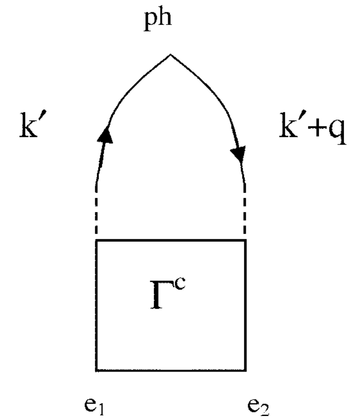

FIG. 2. Diagrammatic representation of the electron-phonon vertex $\Gamma(p,q)$. The square represents the charge vertex function Γ^c that renormalizes the electron, the straight line is the one-particle propagator and the dotted line represents the hopping in which we have expanded. In the vertex e_1 an electron of momentum $\mathbf{p}$ arrives and leaves the vertex e_2 with momentum $\mathbf{p}+\mathbf{q}$. In the vertex ph an incoming phonon line with momentum $\mathbf{q}$ is attached.

The function $\Gamma^c(p)$, which is related to the self-energy corrections of the single-particle Green's function via the Ward identities,[17] is obtained by a Bethe-Salpeter equation[18] generalized to the strong-coupling case

$$\Gamma^c(p) = \Gamma_0^c(p) + \sum_{p'} \Gamma_0^c(p')t^2_{\mathbf{p}-\mathbf{p}'}\Pi(p-p')t^2_{\mathbf{p}'}\Gamma^c(p), \tag{7}$$

where Γ_0^c is the bare charge vertex[11] (a summation over spin index is implicit) whose explicit expression is

$$\Gamma_0^c(p) = \langle n_\sigma\rangle^2\left(\frac{1}{i\omega_n + U} - \frac{1}{i\omega_n - U}\right). \tag{8}$$

Finally, $\Pi(p)$ is the polarization function $\Pi(p) = \int dq G_1(p+q)G_1(q)$. Let us note that compared to the weak-coupling approaches the bare vertex in (7) is a cumulant, i.e., an effective retarded interaction, in place of the bare coupling U.[11] A previous analysis of the charge vertex has revealed that the charge fluctuations become critical at zero temperature for a critical value of the doping and of the Coulomb interaction (δ_c, U_c), signaling an instability towards phase separation at zero momentum.[11] In proximity of the instability the low-energy behavior of the charge vertex is given by

$$\Gamma^c(\mathbf{q}, \omega \sim 0) \simeq -\frac{1}{M(\delta,U,T) + \alpha\mathbf{q}^2 - i\gamma_{\mathbf{q}}\omega}, \tag{9}$$

where $M(\delta,U,T)$ is the mass term, or the inverse squared of the correlation length, that we have found to be a linearly vanishing function of the doping, $\gamma_{\mathbf{q}}$ is the inverse relaxation time of charge fluctuations. Both these functions have been determined numerically in Ref. 11.

As we will show, the proximity to phase separation instability and the softening of the charge fluctuation spectrum at small momentum $\mathbf{q}$ will influence the behavior of the e-ph vertex at finite temperature.

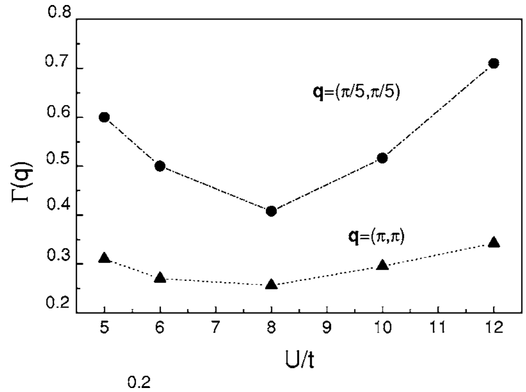

FIG. 3. The electron-phonon vertex $\Gamma(q)$ at varying U/t for $\mathbf{q}=(\pi/5,\pi/5)$ and $\mathbf{q}=(\pi,\pi)$ along the diagonal of the Brillouin zone, while $\mathbf{p}$ is taken on the Fermi surface. The temperature is fixed at $\beta=50/t$, the doping at $\delta=0.12$.

In Fig. 3 we plot the electron-phonon vertex function $\Gamma(p,q)$ at $\mathbf{q}=(\pi/5,\pi/5)$ and at $\mathbf{q}=(\pi,\pi)$ as a function of the Hubbard repulsion U/t ($t=1$ being the energy unit), having fixed $\mathbf{p}$ on the Fermi surface along the $(-1,0)$ direction of the Brillouin zone, $\omega_n=\pi/\beta$, $\beta=1/T=50/t$, and the doping is taken to be $\delta=1-n=0.12$ (see Fig. 4). The phonon frequency is taken to be zero. We note that while for relative small U the el-ph vertex function is decreasing with U, such a behavior has a visible up-turn for values of $U/t\geqslant 8$ at $\mathbf{q}=(\pi/5,\pi/5)$, while being almost constant at $\mathbf{q}=(\pi,\pi)$. The up-turn for $\delta=0.12$ and $U/t\geqslant 8$ can be associated to an incipient transition towards a charge density wave instability.[9]

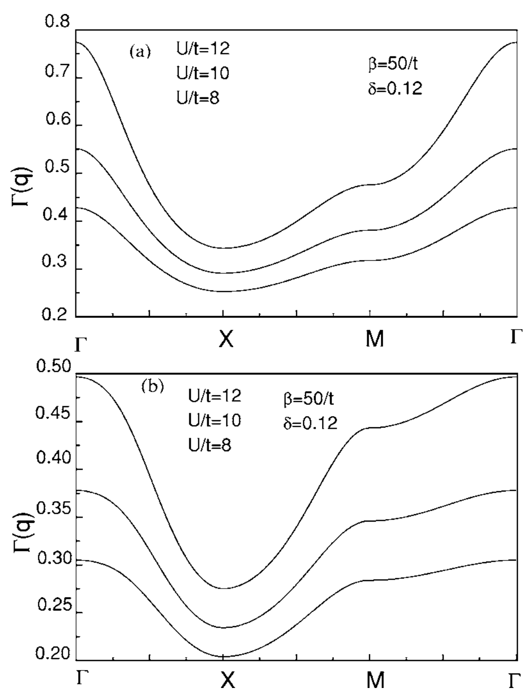

FIG. 4. The electron-phonon vertex $\Gamma(q)$ for scattering electrons on the Fermi surface. Calculations are for the Hubbard model with $t'=0$ (a) and $t'=-0.35t$ (b), the values of the Coulomb interaction are $U/t=12,10,8$ from above. The temperature is fixed at $\beta=50/t$, the doping at $\delta=0.12$.

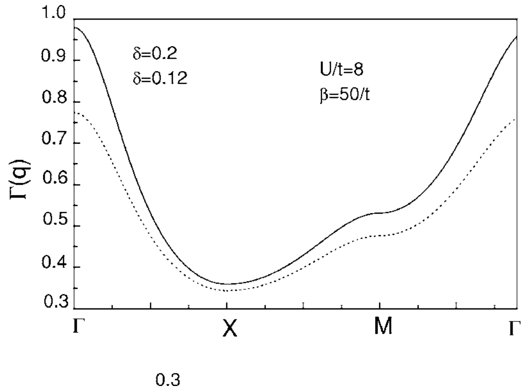

FIG. 5. The electron-phonon vertex for scattering electrons on the Fermi surface. Calculations are for the Hubbard model with $t'=0$, the value of the doping is 0.2 and 0.12 from above. The temperature is fixed at $\beta=50/t$, the Coulomb interaction at $U/t=8$. We find that the vertex function is suppressed with decreasing doping.

The appearance of such instability can also be detected by looking at $\Gamma(p,q)$ plotted as a function of $\mathbf{q}$ along the path $\Gamma=(0,0)\rightarrow X=(\pi,\pi)\rightarrow M=(\pi,0)$ of the first Brillouin zone for the $U-t$ and $U-t-t'$ model. In both cases the data show a pronounced forward scattering peak at $\mathbf{q}=(0,0)$ that increases with U above $U/t\sim 8$. The el-ph vertex is instead suppressed for the backward scattering at $\mathbf{q}=(\pi,\pi)$. This is very similar to what was found in the $1/N$ expansion.[6] The forward scattering peak is also a function of the doping as shown in Fig. 5. Lowering the doping the forward scattering peak decreases implying that also the effective electron-phonon coupling becomes smaller in the low-doping regime.

Coming back to the surprising up-turn of the electron-phonon vertex for intermediate values of U, the results we find are in qualitative agreement with recent QMC and analytical results[8–10] at small momentum. Differently from these approaches the effect of the phase separation in our calculation is relevant in the low-temperature regime below a crossover temperature ($T^{\star}\sim 0.1$). In the slave-boson approaches the increase of the el-ph vertex with U is found only for high temperatures ($kT\sim t$) and is associated to a reentrant behavior to the paramagnetic phase from the phase separation when cooling down the system.[9,10,19] Nevertheless, since slave-bosons approach may have problems at high temperatures, it is not clear if the Hubbard model really shows such a reentrant behavior. In fact, exact numerical calculations are necessary to judge the reliability of the $1/N$ and the Kotliar-Ruckenstein approaches. In order to understand in more details the origin of the phase separation instability as a function of the temperature T, we show in Fig. 6 the charge vertex as a function of $\mathbf{q}=(q,q)$ at different temperatures for $\delta=0.12$. The incipient phase separation is evident below $T/t\simeq 0.1$, above this temperature the charge vertex is insensitive to the increase of T.

In order to assess the importance of the electron-phonon coupling for superconductivity we calculate the renormalization factor

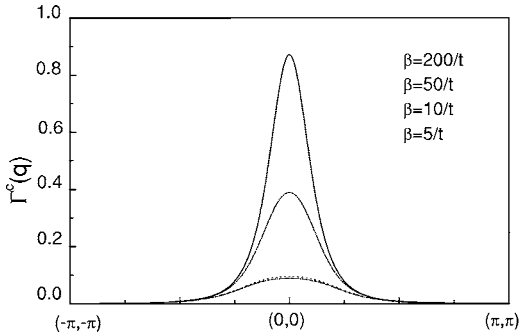

FIG. 6. Charge vertex Γ^c as a function of the temperature, $\beta = 1/T = 200, 50, 10, 5$ from above. The Coulomb interaction is fixed at $U/t = 8$, the doping at $\delta = 0.12$.

$$\Lambda_\alpha = \frac{\int_{FS} \frac{dq}{|\mathbf{v}_q|} \int_{FS} \frac{dq'}{|\mathbf{v}_{q'}|} f_\alpha(\mathbf{q}) g(\mathbf{q}, \mathbf{q}' - \mathbf{q}) f_\alpha(\mathbf{q}')}{\int_{FS} \frac{dq}{|\mathbf{v}_q|} \int_{FS} \frac{dq'}{|\mathbf{v}_{q'}|} f_\alpha^2(\mathbf{q})}, \quad (10)$$

where f_α is the pairing symmetry factor, $f_s(\mathbf{q}) = 1$, $f_{s^\star}(\mathbf{q}) = \cos(q_x) + \cos(q_y)$, $f_{d_{x^2-y^2}}(\mathbf{q}) = \cos(q_x) - \cos(q_y)$, $\mathbf{v}_q$ is the electron velocity, $g(\mathbf{p}, \mathbf{q})$ is the renormalized electron-phonon coupling,

$$g(\mathbf{p}, \mathbf{q}) = \frac{\Gamma(\mathbf{p}, \mathbf{q})}{\sqrt{Z(\mathbf{p}) Z(\mathbf{p} + \mathbf{q})}}, \quad (11)$$

and $Z(\mathbf{p})$ is the wave-function renormalization that can be extracted from the single particle Green's function. In the limit of large Coulomb interaction and in the low-doping regime $Z = A_1^{-1}$ [see Eq. (6)] and is almost a constant $\sim (1 - \langle n_{-\sigma} \rangle)^{-1}$. To analyze the importance of the forward scattering in the transport properties we also calculate the renormalization factor for transport

$$\Lambda_t = \frac{\int_{FS} \frac{dq}{|\mathbf{v}_q|} \int_{FS} \frac{dq'}{|\mathbf{v}_{q'}|} g(\mathbf{q}, \mathbf{q}' - \mathbf{q}) |\mathbf{v}_q - \mathbf{v}_{q'}|^2}{\int_{FS} \frac{dq}{|\mathbf{v}_q|} \int_{FS} \frac{dq'}{|\mathbf{v}_{q'}|} |\mathbf{v}_q|^2}. \quad (12)$$

The results we find are shown in Fig. 7. We find that the s-wave couplings are decreasing functions of U. In the case of nearest-neighbor hopping only, the s-wave couplings are equal since $g_{s^\star}$ is constant on the Fermi surface. Concerning Λ_t, we observe a considerable suppression of this function for large U, reflecting the presence of strong correlations. In fact due to the factor $|\mathbf{v}_q - \mathbf{v}_{q'}|$ the forward scattering contribution is strongly suppressed in Λ_t. The higher d-wave pairing channel is even weaker than Λ_t giving evidence of the fact that, restricting to consider the paramagnetic phase only, the Holstein phonon contribution to superconductivity should be very small.

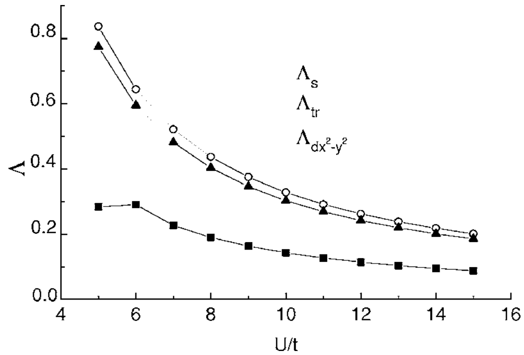

FIG. 7. Renormalization constants Λ_α for different pairing channels and for transport Λ_{tr} relevant for transport for the Hubbard model with $t' = 0$ at increasing U. The temperature is fixed at $\beta = 50/t$, the doping at $\delta = 0.12$.

In conclusion, we have analyzed the influence of charge fluctuations and strong electron correlations on the e-ph vertex in the two-dimensional Hubbard model. The results for the electron-phonon vertex function show an anomalous increase at very small $\mathbf{q}$ as a function of the Coulomb interaction U after an initial decrease, confirming recent numerical and analytical analysis based on QMC and slave-boson approaches. We have shown that the general mechanism responsible for such anomaly can be ascribed to an incipient phase separation and softening of the charge density fluctuation spectrum at low momentum that takes place at a critical value of the Coulomb interaction at fixed doping. Moreover we find that the electron-phonon coupling is enhanced in forward scattering but suppressed for scattering with large momentum transfer by correlations. This implies that, at least in the single band case, the electron-phonon coupling is greatly reduced in transport quantities, consistently with conductivity experiments on high-T_c compounds which do not show any feature associated to phonon scattering.[20] The analysis of the influence of charge fluctuations on the isotope effect and the role of an anisotropic el-ph interaction on the single-particle properties will be the subject of future study.

---

*On leave from Institute of Applied Physics, Chisinau 2028, Moldova.

[1] A. Lanzara *et al.*, Nature (London) **412**, 510 (2001).
[2] H. Keller, Physica B **326**, 283 (2003), and references therein.
[3] G.-H. Gweon, T. Sasagawa, S. Y. Zhou, J. Graf, H. Takagi, D.-H. Lee, and A. Lanzara, Nature (London) **430**, 187 (2004).
[4] J. H. Kim, K. Levin, R. Wentzcovitch, and A. Auerbach, Phys. Rev. B **44**, 5148 (1991); J. H. Kim and Z. Tesanovic, Phys. Rev. Lett. **71**, 4218 (1993).
[5] M. Grilli and C. Castellani, Phys. Rev. B **50**, 16880 (1994).
[6] R. Zeyher and M. L. Kulić, Phys. Rev. B **53**, 2850 (1996).
[7] N. Bulut and D. J. Scalapino, Phys. Rev. B **54**, 14971 (1996).
[8] Z. B. Huang, W. Hanke, E. Arrigoni, and D. J. Scalapino, Phys. Rev. B **68**, 220507(R) (2003).

[9] E. Cappelluti, B. Cerruti, and L. Pietronero, Phys. Rev. B **69**, 161101(R) (2004).
[10] E. Koch and R. Zeyher, Phys. Rev. B **70**, 094510 (2004).
[11] R. Citro and M. Marinaro, Eur. Phys. J. B **20**, 343 (2001).
[12] M. I. Vladimir and V. A. Moskalenko, Theor. Math. Phys. **82**, 301 (1990); V. A. Moskalenko and L. Z. Kon, Condens. Matter Phys. **1**, 23 (1998).
[13] W. Metzner, Phys. Rev. B **43**, 8549 (1991).
[14] See also S. Pairault, D. Senechal, and A.-M. S. Tremblay, Phys. Rev. Lett. **80**, 5389 (1998).
[15] R. Citro and M. Marinaro, Eur. Phys. J. B **28**, 55 (2003).
[16] J. Hubbard, Proc. R. Soc. London, Ser. A **278**, 238 (1963).
[17] J. C. Ward, Phys. Rev. **78**, 182 (1950).
[18] V. M. Galitskii, JETP **34**, 279 (1958).
[19] S. Onoda and M. Imada, cond-mat/0304580 (unpublished).
[20] For example see, H. Takagi, B. Batlogg, H. L. Kao, J. Kwo, R. J. Cava, J. J. Krajewski, and W. F. Peck, Phys. Rev. Lett. **69**, 2975 (1992).