Comment on “Electron-phonon Vertex in the Two-dimensional One-band Hubbard Model”

In the past months a variety of experiments have pointed out an important role of the electron-phonon (el-ph) interaction in many physical properties of the cuprates. These recent findings have triggered a renewed interest for a theoretical understanding of the electron-phonon properties in strongly correlated systems.

One of the most remarkable effects of the strong electronic correlation on the el-ph properties is a to favor forward (small $q$) scattering in the electron-phonon vertex, $q$ being the exchanged phonon momentum. This feature was investigated in the past by means of analytical techniques based on slave-bosons or Hubbard $X$-operators. The assumption of forward scattering predominance within an el-ph framework was shown to explain in a natural way several anomalous properties of cuprates as the difference between transport and superconducting regime and it could be associated to the tendency towards a phase-separation instability.

Our technical approach was based on the four slave-boson method first introduced in Ref. [12]. The electron-phonon vertex function for a finite $U$ Hubbard model has been evaluated as linear response to an external field coupled with charge density. In the spirit of functional integral representation the screening of the electron-phonon function is due to the Gaussian fluctuations of the auxiliary boson fields around the mean-field solution. A similar study at finite $U$ was introduced by A. Lavagna who however did not addressed the momentum modulation of the electron-charge density response. A different choice for the renormalization of the $x_{i}$-operators was in addition done in comparison with Refs. [13, 14] to avoid unphysical divergences in the electron-slave boson matrix elements. Technical details will appear in Ref. [12].

Based on this analytical approach, we can now evaluate the electron-phonon function with the same physical parameters of Ref. [10], namely $n = 0.88$, $\beta = 2$, where $n$ is the electron filling and $\beta = t/k_{B}T$ the inverse temperature in unit of the nearest neighbor hopping parameter $t$.

As only slight difference with respect to Ref. [11] we assume the incoming electron momentum $p$ to be averaged over the Fermi surface and the exchanged frequency to be exactly zero. These marginal differences are expected to not significantly affect the comparison between our results and Ref. [10].

In Fig. 1 we plot the electron-phonon vertex function $g(q)$ at $q = (\pi/4, \pi/4)$ and $q = (\pi, \pi)$ as function of the Hubbard repulsion $U$ for $n = 0.88$ and $\beta = 2$. For $q = (\pi/4, \pi/4)$ we note that while for relatively small $U$ the el-ph vertex function is steadily decreasing with $U$, such a behaviour has an upturn for $U \approx 8$ until a divergence occurs for $U_{c} \approx 9.3$. According this view one is attempted to associate the upturn of $g(q)$ as function of $U$ as an incipient transition towards some charge instability. Note also that for $q = (\pi, \pi)$ no charge instability is observed.

The appearance of charge instability can be also detected by looking at $g(q)$ plotted as function of $q$ ($q = (q,q)\pi$). The evolution of $g(q)$ by varying the Hubbard repulsion $U$ is shown in Fig. 1.b, where we see that the el-ph vertex function is initially suppressed at small $q$ by increasing $U$ (panel b), then it increases as function of $U$ (panel c) until a divergence is established. Note that for $U = 9$ a lattice instability already occurs although for a $q \approx 0.2$ less than $q \approx 1/4$. This reflects the fact that a instability for $q = 0$ (phase separation) is first onset for some critical value of $U$, and then the vector instability is gradually shifted by further increasing of $U$. In
this perspective it is not surprising that momenta on the Brillouin zone edge \( q = (\pi, \pi) \) are less sensitive to the increase of \( U \).

The similarity between our findings and the Quantum Monte Carlo analysis suggests that also the upturn of \( g(q) \) as function of \( U \) reported in Ref. \[10\] could be related to the same tendency towards phase separation or charge instabilities. This does not imply however that phase separation is effectively established, and it should be remarked that the actual occurrence of phase separation in the Hubbard model is still object of debate \[15\].

On one hand expansions around the mean-field solution even including Gaussian fluctuations could enforce unphysical instabilities which could disappear once higher order fluctuations are taken into account, especially in two dimensional systems. On the other hand, small size cluster effects \( (L \times L) \) and large temperature effects in Ref. \[10\] question in principle the generalization of the QMC results in the thermodynamic limit \( (L \rightarrow \infty) \) and at low temperatures. Our results should thus viewed as analytical indications which can trigger further numerical work.

As a final step, we can also employ our slave-boson analysis to extend the range of investigation in regions of parameters not addressed in Ref. \[10\]. In particular we show that a crucial role is played by the temperature that is limited in QMC techniques by the sign problem and by the requirement to be larger that the energy spectrum discretization.

In Fig. 2 we report the dependence of the el-ph vertex function \( g(q) \) at \( q = (\pi/4, \pi/4) \) as varying \( U \) in the large \( (\beta = 2) \) and small \( (\beta = 50) \) temperature limit. As a surprising result, no charge instability is found in the low temperature regime in the contrast with the high temperature range \( (\beta = 2) \). Some conclusions hold true for the phase separation \( q = 0 \) instability (not shown in figure). This results in thus compatible with the absence of phase separation at zero or low temperature.

In order to understand in more detail the origin of the phase separation instability as function of the temperature \( T \) we show in Fig. 2 the phase diagram in the \( T \) vs. \( U \) space with respect to phase separation \( (q = 0) \) and to charge ordering \( (q = (\pi/4, \pi/4)) \). As above mentioned, a phase separation instability occurs in our slave-boson calculations only above a certain temperature \( T/t \gtrsim 0.2 \) \((\beta \lesssim 5)\) \[15\]. As expected, finite \( q \) instability, in the ab-

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**FIG. 1:** (a): Electron-phonon vertex \( g(q) \) as function of the Hubbard repulsion \( U \) for \( q = (\pi/4, \pi/4) \) and \( q = (\pi, \pi) \). The temperature was set here \( \beta = 2 \) and the electronic filling \( n = 0.88 \). (b)-(c) Plot of \( g(q) \) as function of \( q = (q,q)\pi \) for \( U = 2, 4, 6 \) (respectively circles, squares and diamonds in panel b) and for \( U = 7, 8, 9 \) (respectively crosses, triangles up and triangles down in panel c).

**FIG. 2:** (a): Electron-phonon vertex \( g(q) \) at \( q = (\pi/4, \pi/4) \) as function of the Hubbard repulsion \( U \) for \( \beta = 2 \) and \( \beta = 50 \). Electronic filling \( n = 0.88 \). (b) Phase diagram for phase separation \( (q = 0) \) and for the charge ordering \( q = (\pi/4, \pi/4) \) instability in the \( T-U \) space. The dashed line represent the band narrowing factor \( Z \) corresponding to the phase separation instability line.
sence of any long-range Coulomb repulsion, is prevented by the occurrence of phase separation at $q = 0$ in the whole phase space. A interesting insight comes from the comparison of the critical temperature $T_c$ at which the instability towards phase separation occurs with the band narrowing factor $Z$ due to the correlation effects (dashed line in Fig. 2b). The similar dependence on $U$ of $T_c$ and $Z$ points out that the onset of phase separation by increasing temperature is ruled by the comparison between the temperature $T$ and the effective bandwidth $W = Zt$ energy scales. In particular phase separation is established when $T$ become is of the same order of with $Zt (= W/8)$. Once again we stress that the phase separation instability found by our slave-boson calculations which include Gaussian fluctuations could be washed out when higher order fluctuations are taken into account, so that it should be regarded as indicative of tendency towards this kind of instability. Numerical work based on Quantum Monte Carlo techniques will help to answer about the effective role of phase separation or charge ordering in the Hubbard model.

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\( T/t, Z \)

- \( q = (0,0) \)
- \( q = (\pi/4, \pi/4) \)
- \( Z \)

(b)
