Pairing and polarization in systems with retarded interactions

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(Dated: January 28, 2019)

PACS numbers: 71.38.-k, 71.30.+h, 71.10.Fd

Boson-mediated attractive interactions are known to drive instabilities toward broken symmetry phases like charge ordering and superconductivity in electronic systems. The crossover from weak to strong coupling has been extensively studied in both superconducting\textsuperscript{1,2} and charge ordered phases\textsuperscript{1} and\textsuperscript{2}, uncovering a general weak-to-strong coupling scenario in which at weak coupling pairing and condensation occur at the same temperature scale while at strong coupling pairing occurs at a higher temperature than condensation, leading to an intermediate phase of incoherent pairs.

The same evolution from weak to strong coupling in the normal phase has been studied mainly in the limit of instantaneous attraction (attractive Hubbard model), where the above pairs have been proposed to describe the pseudogap regime of the cuprates. This issue, relevant also for other field of applications such as the negative $U$ localizing centers\textsuperscript{3,4}, is in its nature quite hard to attack. In fact, the intermediate regime, in which the system changes its nature from a Fermi liquid to a paired state, intrinsically requires non-perturbative approaches.

The Dynamical Mean Field Theory (DMFT) emerged in the last decade as one of the most successful approaches to deal with non-perturbative regimes. In analogy with classical mean-field, DMFT obtains an exact solution for local quantum dynamics at the expense of spatial fluctuations which are frozen, and becomes exact for large coordination.\textsuperscript{2} DMFT has been successfully applied to the study of the Mott-Hubbard transition in the repulsive Hubbard model, in which by increasing the Coulomb repulsion, a metal becomes a Mott insulator formed by a collection of localized spins. Since the half-filled repulsive and attractive Hubbard model can be mapped one onto the other by a unitary particle-hole transformation on one spin species,\textsuperscript{1} the Mott-Hubbard transition maps onto an analogous metal-insulator transition of the attractive model, where the insulating phase is made of local pairs and empty sites. This means that much of the knowledge we have on the Mott transition can be used for the study of the pairing transition of the attractive model\textsuperscript{1,2,4}. More precisely, we know that the transition is a first order line in the interaction-temperature diagram, ending in a finite temperature critical point\textsuperscript{3}. For temperatures larger than the critical temperature, a crossover between two phases with different properties survives.

This paper is mainly devoted to discuss how such a scenario in enriched when the attraction (or equivalently the repulsion) has a finite intrinsic energy scale, given by the bare frequency of the boson which mediates the attraction. The pairing process, which becomes a bipolaronic transition when the mediator boson is a phonon, survives the inclusion of boson dynamics, and it has been studied within DMFT by various authors\textsuperscript{2,4,6}. The new energy scale given by the intrinsic frequency for the boson dynamics has to be compared with both the temperature and the electron half-bandwidth $D$. The most interesting region, in which the use of DMFT is crucial, is the intermediate region in which none of the energy scale and the temperature are negligible. The ratio $\gamma = \omega_0/D$ between the boson energy and the electron hopping energy naturally defines an adiabatic regime in which $\gamma$ is small and the electronic degrees of freedom are much faster than bosonic ones. In this regime a gradual increase of the coupling determines a crossover from quasi-free electrons to almost localized “polarons”, quasiparticles in which the electrons are strongly bound to the bosonic degrees of freedom thereby determining a polarization of the boson field which couples to the electron density. Such a crossover can be unambiguously defined by looking at the polarization properties of the boson field\textsuperscript{3,10}. In the opposite antiadiabatic limit, in which the boson dynamics is faster than the electronic one, the interaction becomes instantaneous, and we recover either the attractive or repulsive Hubbard models.

The main result of this work is to clearly disentangle...
the polarization and the pairing crossovers in the normal phase and to define unambiguously also the pairing crossover. We find that, the larger is $\gamma$, the more the two processes occur at different coupling, opening an interesting regime in between.

Although we do not need to specify the physical origin of the bosonic mediator, we consider for the sake of definiteness the Holstein model which describes tight-binding electrons coupled to dispersionless Einstein phonons. Within DMFT the lattice Holstein model is mapped onto a local impurity problem whose action reads:

$$S_{el} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^\dagger(\tau)G_0^{-1}(\tau - \tau')c_\sigma(\tau')$$

$$S_{ph} = \frac{1}{2} \int_0^\beta d\tau \left( \frac{\dot{x}^2(\tau)}{\omega_0^2} + x^2(\tau) \right)$$

$$S_{el-ph} = -\sqrt{U} \int_0^\beta d\tau x(\tau) \left( n(\tau) - 1 \right)$$

where $n(\tau) = \sum_\sigma c_\sigma^\dagger(\tau)c_\sigma(\tau)$. We take $\kappa = m\omega_0^2 = 1$, $m$ being the mass of the oscillator. In Eq. $S_{el}$ $G_0^{-1}(\tau)$ is the bath propagator that has to be evaluated self-consistently [2]. The self-consistency condition which enforces the DMFT contains the informations about the original lattice, and for the infinite coordination Bethe lattice we consider it takes the simple form $G_0^{-1}(\tau) = -\partial_x + (D^2/4)G(\tau)$ where $G(\tau)$ is the local Green’s function and $D$ is the half-bandwidth. For our model with dispersionless Einstein modes, the phononic degrees of freedom are not subject to an analogous self-consistency. Since the action is manifestly particle-hole symmetric, it describes a half-filled system with density $n = 1$. In the antiadiabatic limit ($\omega_0 = \infty$, $U$ finite) the kinetic term of the boson field vanishes, the interaction becomes therefore instantaneous and the action coincides with that of an attractive Hubbard model after an Hubbard-Stratonovich (HS) decoupling of the quartic interaction term. We notice incidentally that under the transformation which maps the attractive Hubbard model on the repulsive one, $S_{el-ph}$ becomes

$$S_{el-ph} = -\sqrt{U} \int_0^\beta d\tau x(\tau) \left( n_\uparrow(\tau) - n_\downarrow(\tau) \right)$$

which, once the spin index is interpreted as an orbital one, has been studied in Ref. [11] to describe the Jahn-Teller (JT) coupling in manganites.

An efficient method to solve (1,2,3) at finite temperature is the Quantum Monte Carlo method (QMC) in the Blankenbecler-Scalapino-Sugar (BSS) approach [12]. This method works well in the range of temperatures we are interested in (i.e. not too low temperatures) and naturally yields electronic and bosonic correlation functions, as well as the probability distributions associated to the boson fields. The method is not affected by the negative sign-problem, and its main limitation comes in the adiabatic regime ($\gamma \ll 1$) where the boson becomes heavy making more difficult to sample correctly the available phase space. In the BSS scheme the fermions are integrated out, and the bosons coordinates $x(\tau)$ are discretized into $L$ imaginary-time slices of width $\Delta \tau = \beta/L$ and then sampled by the Monte Carlo simulation. $L$ has to be chosen large enough to reduce as much as possible $\Delta \tau$, which controls the the Trotter discretization error. To keep $\Delta \tau$ less than 1/8 we used 32 slices except for the lowest temperature ($\beta = 8$) for which we have used $L = 64$. As customary, the statistical error is reduced by dividing measurements in bins. The self-consistency is achieved in a few DMFT iterations, typically from 5 to 10, depending on the values of the parameters $[4]$.

Now we introduce the key quantities we employ for the characterization of pairing and polarization and their temperature dependence. Namely, we compute the probability distributions of the endpoint

$$P(X) = \left( \delta(X - x(0)) \right)$$

and of the center of mass $X_c$ ("centroid") of the boson path in imaginary time

$$P(X_c) = \left( \delta(X_c - 1/\beta \int_0^\beta x(\tau)d\tau) \right)$$

where the averages are evaluated over the action given by Eqs. (1-3).

The first quantity has a rather straightforward meaning as a probability distribution of the lattice displacement (if the boson is thought as a phonon). If $P(X)$ has a single maximum, corresponding to a uniform displacement of the field, the system is not polarized. A lattice polarization reflects in the presence of two maxima in $P(X)$, corresponding to opposite polarization of occupied and unoccupied sites (bimodal behavior) [10]. In this way a qualitative difference is identified between the polarized and unpolarized regimes, which allows for unambiguous way to draw a crossover line, as opposed to estimates based on smoothly varying functions as average lattice fluctuations or electron kinetic energy.

The meaning of the centroid variable $X_c$ has been discussed in [13] for a single particle in a binding potential. Here the variable $X$ represents the position of the particle, and $X_c$ is the classical position of the particle [13]. For an heavy particle, the classical limit holds, so that $X$ and $X_c$ coincide [13]. As the particle is made lighter, the wave function becomes broader, increasing the variance of $P(X)$ while $P(X_c)$ turns out to be essentially determined by the binding range of the potential. Here, we use $P(X_c)$ for the many-body problem, and propose that pairing, i.e., the formation of local pairs, can be associated with a development of a multimodal behavior in our centroid distribution $P(X_c)$. This estimator of the pairing crossover has the same advantage of the previous one,
and it finally allows us to draw, beside the polarization line $U_{\text{pol}}$, an equally unambiguous pairing line $U_{\text{pair}}(T)$ for any value of the boson frequency. A crossover line can also be associated with maxima of susceptibilities related to the relevant quantity, e.g., the electron-phonon correlation function in the case of polaron crossover [14]. However, this choice is not obvious in the case of pairing, where charge, superconductivity or Pauli [15] susceptibilities can play this role. We defer a comparison with these methods in the concluding remarks.

The ability of our estimator to determine the pairing crossover can be understood by considering directly the interaction term $\gamma$ in the action. In the adiabatic limit ($\gamma \to 0$) the kinetic term forces the boson path to be $\tau$-independent. The boson field becomes classical and the interaction term can be written as $-\sqrt{U}X \int_0^\beta d\tau (n(\tau) - 1)$, where $X$ indicates the constant value assumed by $x(\tau)$ along the whole imaginary time path. In this limit the centroid coordinate $X_c$ is equal to $X$ and the two distributions $P(X)$ and $P(X_c)$ obviously coincide. Thus the centroid distribution becomes bimodal when the system is polarized, which is exactly what one expects in the static limit, since a static field can induce pairing only with a finite polarization.

On the other hand, in the opposite atomic ($D \to 0$, $\gamma \to \infty$) limit the electron density becomes a constant of motion. Therefore Eq. (4) takes the transparent form $-\sqrt{U} (n - 1) \int_0^\beta dx x(\tau)$ where the electron density is directly coupled to the centroid $X_c$. The average appearing in Eq. (5) is readily carried out, giving

$$P(X_c) \propto \exp \left[ -\beta \left( \frac{X_c^2}{2} - \frac{1}{\beta} \log(2 \cosh(\beta \sqrt{U} X_c + 1)) \right) \right]$$

which becomes bimodal for $T < U/2$. This is exactly the scale where double occupancies start to proliferate in the atomic limit. Therefore the bimodality of $P(X_c)$ correctly signals the onset of pairing also in the adiabatic regime. In the same limit, it can be proved that the endpoint distribution $P(X)$ has a variance which scales with $1/\sqrt{\Delta \tau}$ and as a consequence no definite polarization may occur. We finally notice that the $D \to 0$ limit of adiabatic $P(X)$ coincides with $P(X_c)$ of Eq. (5).

Since for $\omega_0 = 0$ the distributions of $X$ and $X_c$ coincide, we conclude that in the atomic limit the $P(X_c)$ is the same for $\omega_0 = 0$ and $\omega_0 = \infty$. This suggests that the pairing crossover may depend on $\omega_0$ more weakly than the polarization one.

To analyze the evolution of $P(X)$ and $P(X_c)$ at finite $D$ and $\omega_0$ we use BSS-QMC. The numerically exact results, shown in Fig. 1, clearly show that $P(X)$ and $P(X_c)$ tend to coincide in the relatively adiabatic case $\gamma = 0.1$, as expected from the previous arguments about the adiabatic limit. The two quantities are clearly different for $\gamma = 1$ and 8. Actually for temperatures smaller than $\omega_0$, the polarization crossover $U_{\text{pol}}$ moves to larger values as $\gamma$ is increased, while the line $(U_{\text{pair}})$ where $P(X_c)$ becomes bimodal is only slightly shifted to larger couplings with increasing $\gamma$. This is strongly reminiscent of the behavior of the metal-insulator transition in the Holstein model at $T = 0$, whose critical coupling is slowly increasing with $\gamma$ and then saturates to the asymptotic $\gamma = \infty$ value [5]. On the other hand, the polarization crossover is almost directly proportional to $\gamma^2$. Both at zero and at finite temperature the line where the centroid becomes bimodal does not coincide with the metal-insulator line, but it can be considered a precursor which depends in a very similar way on $\gamma$ and on $U/D$.

Our DMFT results can also be compared with the semi-analytical results for $\gamma = 0$ [10], which is represented by the green dashed line in Fig. 1. It can be seen that the $\gamma = 0.1$ case is in very good agreement with the adiabatic result, and also the $\gamma = 1$ and 8 cases, at high temperature, fall on the same curve. It must be observed also that, in the full DMFT calculation, the centroid distribution depends weakly on $\gamma$, as suggested by the atomic limit. Interestingly, the adiabatic result displays a re-entrance at low temperatures. Although the QMC simulations do not reach sufficiently low temperatures, we find that the re-entrance is present also for $\gamma$ different from zero, as indicated by the arrows in Fig. 1 which mark $T = 0$ results for the polarization crossover for the Holstein model [7]. This phenomenon has been also reported for the Mott transition in the repulsive model [16], and associated to spin entropy of the insulator. The same physics holds here, where the entropy is associated
to a pseudo-spin.

A strong indication that the centroid distribution marks the pairing crossover is provided by the analysis of the double occupancies \(|n_{\uparrow}n_{\downarrow}|\). This quantity increases from the non-interacting value 1/4 to the asymptotic value of 1/2 as the coupling is increased. We computed \(|n_{\uparrow}n_{\downarrow}|\) for different temperatures in the antiadiabatic regime \(\gamma = 8\), chosen in order to have clearly different values for \(U_{\text{pol}}\) and \(U_{\text{pair}}\). We notice that our results are correctly close to the attractive Hubbard model.\(^{17}\)

In Fig. 2 \(U_{\text{pol}}\) and \(U_{\text{pair}}\) are marked, respectively, by a black solid square and a blue solid circle, for each temperature. \(|n_{\uparrow}n_{\downarrow}|\) at \(U_{\text{pol}}\) is rapidly increases with decreasing temperature, while \(|n_{\uparrow}n_{\downarrow}|\) calculated at \(U_{\text{pair}}\) is almost constant with temperature, or even slightly decreasing at low \(T\). So, when the centroid distribution becomes multimodal, the double occupancies are approximately 70% of the saturation value of 1/2. Similar results are found also for \(\gamma = 1\) and 0.1, where it is however harder to distinguish \(U_{\text{pair}}\) from \(U_{\text{pol}}\). This establishes the efficiency of our centroid distribution in pinpointing the pairing crossover for the whole range of parameters.

In conclusion for a half-filled system subject to retarded attractive (repulsive) interaction we observe three qualitatively different behaviors \(i)\) a normal state of delocalized particles, \(ii)\) a pair region of bounded incoherent pairs with no associated polarization, \(iii)\) a bipolaron region in which pairing is associated with a definite polarization. These three regions are delimited by two clear cut lines where the probability distributions for the centroid and for the endpoint of the bosonic path, develop a bimodal shape. While the border between the normal and the local pair phase is weakly dependent on the adiabatic ratio, the one between the pair and the bipolaronic phase, shifts to higher value of the coupling with increasing \(\gamma\), so that the pair phase gets larger, eventually covering the whole right hand part of the phase diagram in the attractive Hubbard limit \((\gamma = \infty)\). The \(U_{\text{pair}}\) line is very similar to the \(T^*\) line found in Ref.\(^{\text{[13]}}\) by looking at the maximum of the spin susceptibility. For temperatures of the order of \(\omega_0\) the two lines merge because phonons at such temperatures behaves classically. Finally, due to the electron-hole symmetry the retarded attractive interaction is mapped onto a JT model leading to an Hubbard-like repulsion in the antiadiabatic limit. In this case the crossover at \(U_{\text{pair}}\) is associated to the formation of local orbital ordering for JT interactions. The crossover at \(U_{\text{pol}}\) survives only in the retarded JT case and is shifted toward higher value of the coupling as the phonon frequency increase leaving a region in which orbital ordering is not associated with JT polarons.

We acknowledge useful discussions with C. Castellani and A. Toschi. This work was supported by MIUR-Cofin 2003 matching funds programs.

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