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### Abstract

We examine the superconducting solution in the Hubbard-Holstein model using Dynamical Mean Field Theory. The Holstein term introduces the site-independent Boson fields coupling to local electron density, and has two competing influences on superconductivity: The Boson field mediates the effective electron-electron attraction, which is essential for the S-wave electron pairing; the same coupling to the Boson fields also induces the polaron effect, which makes the system less metallic and thus suppresses superconductivity. The Hubbard term introduces an energy penalty  $U$  when two electrons occupy the same site, which is expected to suppress superconductivity. By solving the Hubbard-Holstein model using Dynamical Mean Field theory, we find that the Hubbard  $U$  can be beneficial to superconductivity under some circumstances. In particular, we demonstrate that when the Boson energy  $\omega$  is small, a weak local repulsion actually stabilizes the S-wave superconducting state. This behavior can be understood as an interplay between superconductivity, the polaron effect, and the on-site repulsion: As the polaron effect is strong and suppresses superconductivity in the small  $\omega$  regime, the weak on-site repulsion reduces the polaron effect and effectively enhances superconductivity. Our calculation elucidates the role of local repulsion in the conventional S-wave superconductors.

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# The role of local repulsion in superconductivity in the Hubbard-Holstein model

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We examine the superconducting solution in the Hubbard-Holstein model using Dynamical Mean Field Theory. The Holstein term introduces the site-independent Boson fields coupling to local electron density, and has two competing influences on superconductivity: The Boson field mediates the effective electron-electron attraction, which is essential for the S-wave electron pairing; the same coupling to the Boson fields also induces the polaron effect, which makes the system less metallic and thus suppresses superconductivity. The Hubbard term introduces an energy penalty  $U$  when two electrons occupy the same site, which is expected to suppress superconductivity. By solving the Hubbard-Holstein model using Dynamical Mean Field theory, we find that the Hubbard  $U$  can be beneficial to superconductivity under some circumstances. In particular, we demonstrate that when the Boson energy  $\Omega$  is small, a weak local repulsion actually *stabilizes* the S-wave superconducting state. This behavior can be understood as an interplay between superconductivity, the polaron effect, and the on-site repulsion: As the polaron effect is strong and suppresses superconductivity in the small  $\Omega$  regime, the weak on-site repulsion reduces the polaron effect and effectively enhances superconductivity. Our calculation elucidates the role of local repulsion in the conventional S-wave superconductors.

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## I. INTRODUCTION

The superconductors are typically classified as being “conventional” and “unconventional”. For conventional superconductors, the electron pairing is mediated by some external Boson field (phonons for example), and the strength of electron-electron interaction energy is relatively small compared to the (renormalized) electron band energy. This class of superconductors can be properly described by Bardeen-Cooper-Schrieffer theory [1–3], where phonons are not explicitly included, or by a more realistic Eliashberg theory [4–10], where the electron-phonon, electron-electron, electron-impurity (disorder in the lattice) interactions are all taken into account by self-consistently keeping their respective low-order diagrammatic contributions to self energies [6, 7, 10]. The Eliashberg theory can be regarded as a self-consistent perturbation theory, and it is the “weakly correlated” nature [11] of the problem that makes the perturbation a reasonable approximation. For unconventional superconductors, the electron pairing is believed to originate from the electron-electron interaction [12–14], although the understanding is still far from being complete [15]. The unconventional superconductors include the layered materials such as cuprates [16, 17] and iron-based materials [18–20]. The multi-orbital and “strongly correlated” nature make the system intrinsically complicated – there are many competing symmetry-breaking phases [12, 21]; even if the zero-temperature state can be identified, a proper description of the excitations (therefore properties at non-zero temperatures) is still highly non-trivial [22–25]. We note, however, that the recent experiments of mono-layer FeAs on SrTiO<sub>3</sub> substrate strongly suggests the importance of the Boson contribution (an interfacial optical phonon mode) to superconductivity [20, 26–28].

The Hubbard-Holstein model is the simplest model that captures the physics of “conventional” electron pairing and the Coulomb repulsion. The Holstein term [29] introduces the site-independent Boson fields coupling to local electron density, which has two competing effects on superconductivity. On the one hand, the Boson field mediates the effective electron-electron attraction, which is essential for the S-wave electron pairing; on the other hand, the coupling to the Boson fields “drags” the electron motion, which makes the system less metallic (polaron effect) [30–34] and thus suppresses superconductivity. For the Holstein model at strong electron-Boson coupling regime, the Migdal-Eliashberg (ME) theory [4, 5] leads to the superconducting ground state at zero temperature for all Boson energies  $\Omega$  [35]; whereas the Dynamical Mean Field Theory (DMFT) [36–39], which is non-perturbative and becomes exact in the infinite dimension limit, leads to the polaron insulating state at small  $\Omega$  and the superconducting state

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at large  $\Omega$  [35]. The discrepancy in the small  $\Omega$  regime is attributed to the underestimation of polaron effect in the ME theory [40, 41]. The Hubbard term [42] introduces an energy penalty  $U$  when two electrons occupy the same site, which generally favors the formation of local moments (i.e. one electron occupies one of two local spin orbitals). For symmetry-breaking phases, the Hubbard term can lead to ferromagnetism [25], anti-ferromagnetism [43, 44], stripe phase [45], and even  $d$ -wave superconductivity [46, 47]; without long-range magnetic orders, the Hubbard term can result in a Mott insulating phase [36, 48, 49].

From the perspective of competing ground states, the Hubbard-Holstein model deals with the interplay between superconductivity, polaron, and Mott physics. Among these three phases, the superconducting and Mott insulating phases exclude each other, as the former needs an effective electron-electron attraction, whereas the latter requires a large local repulsion. The polaron effect is, however, always present. The studies on the Hubbard-Holstein model are mostly from the “strongly correlated” point of view: Starting from a (nearly) Mott insulating phase, how does the polaron modify the electronic behavior [40, 41, 50–53]? In this work, we approach this problem from the complementary “weakly correlated” point of view: Starting with a superconducting or polaron insulating phase, what is the effect of the on-site repulsion? Generally, the on-site repulsion is expected to suppress the S-wave superconductivity. By explicitly solving the Hubbard-Holstein model using DMFT, we find the above statement requires some explanations. We explicate this statement as follows: At a given electron-Boson coupling, the on-site repulsion suppresses the S-wave superconductivity in the sense that the Hubbard  $U$  reduces the largest possible value of the superconducting gap; however, it is beneficial to superconductivity when the polaron effect is strong. A simple picture will be provided to explain this finding and to clarify the role of on-site repulsion. The rest of the paper is organized as follows. In Section II we describe the model and the method we use. In Section III we present our results and discuss what they imply. A brief conclusion is given in Section IV.

## II. MODEL AND METHOD

The Hubbard-Holstein model is given by

$$H = H_{elec} + H_{hub} + H_{ph} + H_{e-ph} \quad (1)$$

with  $H_{elec} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}$ ,  $H_{hub} = U \sum_i c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}$ , and  $H_{ph} + H_{e-ph} = \Omega \sum_i a_i^\dagger a_i + g \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i,\sigma} - 1)(a_i + a_i^\dagger)$ . Here  $c_{\mathbf{k},\sigma}/c_{i,\sigma}$  represents the Fermion degree of freedom in the momentum/real space, and  $a_i$  represents the local Boson degree of freedom. We consider the conduction band of semicircular density of states (DOS)  $\nu(\varepsilon) = \sqrt{4t^2 - \varepsilon^2}/(2\pi t^2)$ , which corresponds to the Bethe lattice of infinite dimension, a limit where the spatial fluctuations become negligible and the DMFT result becomes exact [36]. We take  $t \equiv 1$ , and all energies including the Hubbard  $U$ , the electron-Boson coupling  $g$ , and the Boson energy  $\Omega$  are all measured in  $t$ . We shall show the results of  $g = 0.6$  and half-filled band, for several Hubbard  $U$ .

The model is solved using DMFT, which fully captures the local interaction via an auxiliary impurity model, and determines the impurity-bath hybridization parameters by equating the lattice local Green’s function to the impurity Green’s function. To describe the superconducting solution, the impurity model is

$$H_{imp,SC} = \varepsilon_d \sum_{\sigma} c_{1,\sigma}^\dagger c_{1,\sigma} + \sum_{p=1}^N t_{sc,p} (c_{p,\uparrow}^\dagger c_{p,\downarrow}^\dagger + h.c.) + \sum_{p=2,\sigma}^N t_p [c_{1,\sigma}^\dagger c_{p,\sigma} + h.c.] + \sum_{p=2,\sigma}^N \varepsilon_p c_{p,\sigma}^\dagger c_{p,\sigma} \quad (2)$$

$$+ g(n_{1,\uparrow} + n_{1,\downarrow} - \alpha)(a + a^\dagger) + \Omega a^\dagger a + U c_{1,\uparrow}^\dagger c_{1,\uparrow} c_{1,\downarrow}^\dagger c_{1,\downarrow}$$

Notice that site 1 is the impurity site, and the particle numbers are not conserved via the term  $t_{sc,p}(c_{p,\uparrow}^\dagger c_{p,\downarrow}^\dagger + h.c.)$ . We use exact diagonalization (ED) [54] as the impurity solver, and consider the zero-temperature solution. The computational details are given in Ref. [35, 55], and here we simply point out that the effective temperature needed in the ED solver is chosen as  $T_{eff} = 0.01$ . Using Pauli matrices  $\sigma_i$  ( $i = 1, 2, 3$ ) [56], the Nambu self-energies and lattice Green’s functions obtained in DMFT are parameterized as

$$\begin{aligned} \hat{\Sigma}(i\omega_n) &= i\omega_n[1 - Z(i\omega_n)]\hat{\sigma}_0 + \chi(i\omega_n)\hat{\sigma}_3 + \phi(i\omega_n)\hat{\sigma}_1 \\ \hat{G}^{-1}(\mathbf{k}, i\omega_n) &= \hat{G}_0^{-1}(\mathbf{k}, i\omega_n) - \hat{\Sigma}(i\omega_n) \\ &= i\omega_n Z(i\omega_n)\hat{\sigma}_0 - [\varepsilon_{\mathbf{k}} + \chi(i\omega_n)]\hat{\sigma}_3 - \phi(i\omega_n)\hat{\sigma}_1. \end{aligned} \quad (3)$$

with  $\hat{G}_0(\mathbf{k}, i\omega_n)$  being the non-interacting Green's function. The component associated with  $\sigma_2$  is ignored without loss of generality [10]. We characterize superconductivity by the superconducting gap  $\Delta$ , which can be evaluated from the Green's function as [35]

$$\frac{\Delta}{2} = \frac{\phi(\omega = 0)}{Z(\omega = 0)} \approx \frac{\phi(i\omega_0)}{Z(i\omega_0)}, \quad (4)$$

To simplify notations, we from now on denote  $Z = Z(0) \approx Z(i\omega_0)$  and  $\phi = \phi(0) \approx \phi(i\omega_0)$ . The two quantities appeared in the gap [Eq. (4)] are worth more discussions.  $\phi$  is the off-diagonal component in the self energies which directly relates to superconductivity;  $1/Z$  is the quasi-particle weight which measures the electron density near the Fermi energy. Larger  $Z$  indicates that the system is less metallic and is therefore against superconductivity. As we will see shortly, these two quantities display different responses to the Holstein and Hubbard terms, which is the origin of the non-monotonous behavior of the superconducting gap.

Before presenting our simulations, we discuss some important dimensionless parameters defined in the Hubbard-Holstein model. There are four energy parameters: the half bandwidth  $2t$  (which is also the Fermi energy  $E_F$  for the half-filled band), the electron-Boson coupling  $g$ , the Boson energy  $\Omega$ , and the on-site repulsion  $U$ . As we mainly focus on the “weakly correlated” small  $U$  limit, we first take  $U = 0$ . Based on the ME theory,  $\Omega/(2t)$  ( $= \Omega/E_F$ ) is the small dimensionless parameter [4, 5, 9, 10], and it gives the superconducting solution for all values of  $\Omega$  for a fixed  $g$  [see Fig. 1(a)]. DMFT introduces another dimensionless parameter  $\lambda = g^2/(\Omega t)$  [57], above some critical value the ME theory breaks down [35, 40, 41, 50]. The interpretation of  $\lambda$  is straightforward – it measures how easily the Boson fields can be excited. Large  $\lambda$ , corresponding to the small  $\Omega$  and/or large  $g$ , indicates more Boson quanta are induced. According to DMFT, a superconducting solution is obtained for small  $\lambda$  (large  $\Omega$ ); a polaron insulating phase is stabilized for large  $\lambda$  (small  $\Omega$ ) [35]. The discrepancy between ME theory and DMFT in large  $\lambda$  (small  $\Omega$ ) regime originates from that ME theory underestimates the Boson fluctuations (which is treated exactly in DMFT) and thus the polaron effect [40, 41]. The Hubbard term introduces another dimensionless parameter  $U/t$ . The relative strength between  $U/t$  and  $\lambda$  determines if Hubbard model or the Holstein model should be used as the starting point. When  $U/t \approx \lambda$ , where both terms are important, the behavior may not be easy to expect. DMFT, which is a non-perturbative method, is particularly useful in this situation, as it takes both Hubbard and Holstein terms on the equal footing, and can faithfully describe the behavior in the intermediate regime.

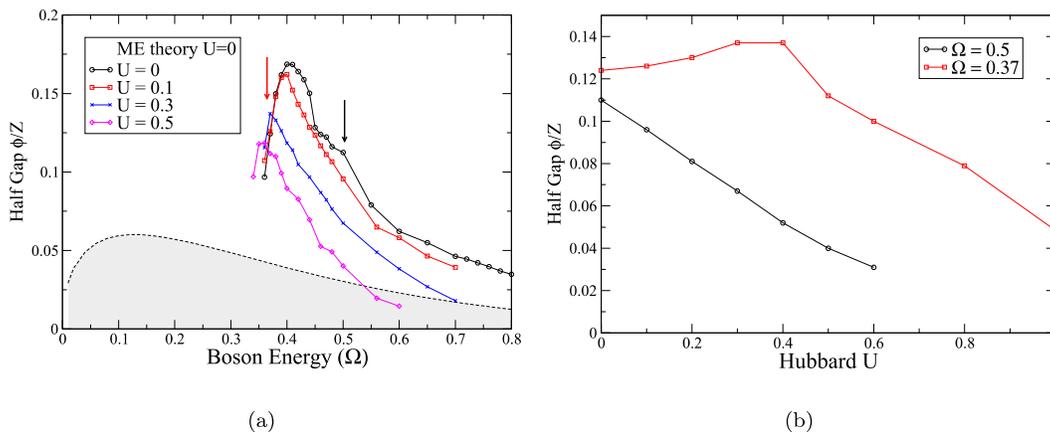


FIG. 1: (a) The half gap as a function of Boson energy at half filling, for several  $U$ . When  $U = 0$ , the optimal Boson energy  $\Omega_{opt}$  has the largest superconducting gap. For  $\Omega > \Omega_{opt}$ , introducing  $U$  always reduces the gap. For  $\Omega < \Omega_{opt}$ , the gap enlarges at small  $U$ , and shrinks at large  $U$ . Increasing Hubbard  $U$  gradually reduces  $\Omega_{opt}$  and the corresponding gap size. The result from ME theory for  $g = 0.6$  is provided in the shaded area as a reference. Two arrows mark two representative  $\Omega = 0.5$  (black) and  $\Omega = 0.37$  (red). (b) The half gap as a function of  $U$ , for two representative  $\Omega = 0.5$  ( $> \Omega_{opt}$ , black) and  $\Omega = 0.37$  ( $< \Omega_{opt}$ , red). For  $\Omega = 0.37$ , a non-monotonous behavior is seen. Their corresponding  $Z$  and  $\phi$  are given in Table I.

### III. RESULTS AND DISCUSSION

$U$	0	0.1	0.2	0.3	0.4	0.5	0.6	3.0	5.0
$\phi$	0.288 (1)	0.23 (0.80)	0.185 (0.64)	0.145 (0.50)	0.106 (0.37)	0.078 (0.27)	0.058 (0.20)	0.0 (0.0)	0.0 (0.0)
$Z$	2.57 (1)	2.41 (0.94)	2.27 (0.88)	2.15 (0.84)	2.05 (0.80)	1.95 (0.76)	1.86 (0.72)	1.86 (0.72)	6.60 (2.57)
$\Delta/2$	0.11 (1)	0.096 (0.87)	0.081 (0.74)	0.067 (0.61)	0.052 (0.47)	0.040 (0.36)	0.031 (0.28)	0.0 (0.0)	0.0 (0.0)

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$U$	0	0.1	0.2	0.3	0.4	0.5	0.6	3.0	5.0
$\phi$	7.465 (1)	6.554 (0.88)	5.214 (0.70)	3.430 (0.46)	2.122 (0.28)	0.824 (0.11)	0.572 (0.08)	0.0 (0.0)	0.0 (0.0)
$Z$	60.05 (1)	52.07 (0.87)	40.01 (0.67)	25.00 (0.42)	15.46 (0.26)	7.38 (0.12)	5.73 (0.10)	1.88 (0.03)	6.55 (0.11)
$\Delta/2$	0.124 (1)	0.126 (1.01)	0.130 (1.05)	0.137 (1.10)	0.137 (1.10)	0.112 (0.90)	0.100 (0.81)	0.0 (0.0)	0.0 (0.0)

TABLE I:  $\phi$  (off-diagonal component in self energies),  $Z$  (inverse of quasi-particle weight), and  $\Delta/2 = \phi/Z$  (half gap), for  $g = 0.6$  and  $U = 0$  to  $0.6$  (small  $U$ ),  $3$  and  $5$  (medium  $U$ ). The upper half corresponds to  $\Omega = 0.5$  ( $> \Omega_{opt}$ ), and the lower half  $\Omega = 0.37$  ( $< \Omega_{opt}$ ). The numbers in parentheses are the ratios normalized to the corresponding  $U = 0$  values. For example, for the  $\phi$  in the  $U = 0.1$  column,  $(0.80) = \phi(U = 0.1)/\phi(U = 0) = 0.23/0.288$  (upper half);  $(0.88) = 6.554/7.465$  (lower half). For  $\Omega = 0.5$ , Hubbard  $U$  simply suppresses the superconducting gap. For  $\Omega = 0.37$ , increasing  $U$  up to  $\sim 0.4$  enhances the superconducting gap, above which superconductivity is suppressed. Notice that the Hubbard  $U$  suppresses both polaron and superconducting effects, but the impacts are different (see the numbers in parentheses). For  $\Omega = 0.5$ , a weak  $U$  mainly suppresses the superconducting effect, therefore reduces  $\Delta$ ; for  $\Omega = 0.37$ , a weak  $U$  mainly suppresses the polaron effect, therefore enhances  $\Delta$ . For both  $\Omega$  at  $U = 3$ , the Hubbard term completely suppresses the superconductivity. Further increasing to  $U = 5$ ,  $Z$  again increases, which is an indication of Mott insulating phase.

We now present our results. The half superconducting gap  $\Delta/2$ , the inverse of quasi-particle weight  $Z$ , and the spectral functions are the quantities we use to characterize the system. Fig. 1(a) shows the (half) superconducting gap as a function of Boson energy at  $U = 0, 0.1, 0.3$  and  $0.5$ . For all values of  $U$  presented here, there exists an optimal Boson energy  $\Omega_{opt}(U)$  for superconductivity, and this optimal energy, as well as the corresponding gap size, decrease as  $U$  increases. In the small  $U$  limit, the system responses to  $\Omega > \Omega_{opt}$  and  $\Omega < \Omega_{opt}$  [ $\Omega_{opt} \equiv \Omega_{opt}(U = 0) \sim 0.4$  from Fig. 1(a)] are different: Introducing a  $U$  in the former regime weakens the superconducting gap; introducing a  $U$  in the latter regime first *enhances* the superconducting gap, and then weakens the superconducting gap. The difference between two responses is more clearly shown in Fig. 1(b), which plots the gap values for two representative  $\Omega = 0.50 > \Omega_{opt}$ ,  $\Omega = 0.37 < \Omega_{opt}$  as a function of  $U$ . From Fig. 1(b), we see explicitly that for  $\Omega = 0.37$ , a weak local repulsion up to  $U \lesssim 0.4$  actually favors superconductivity. The main message from Fig. 1 is that the Hubbard term indeed suppresses superconductivity, in the sense that increasing  $U$  reduces the gap value at  $\Omega_{opt}(U)$ ; at a given Boson energy  $\Omega < \Omega_{opt}$ , however, a weak repulsion stabilizes the superconducting solution.

To understand this behavior, we first recapitulate our understanding on the Holstein model (i.e.  $U = 0$ ), and the following discussion is based on Ref. [35]. For  $U = 0$ , the existence of  $\Omega_{opt}$  can be understood as the competition between the superconducting and the polaron effect at different  $\Omega$  regimes. In the large  $\Omega$  limit, the Boson field plays very little role in the ground state, and both superconducting and polaron effects are negligibly small. In terms of Green's function, it corresponds to  $Z \rightarrow 1$  and  $\phi \rightarrow 0$ . Upon lowering  $\Omega$ , both superconducting and polaron effects enhance, but their increasing rates are different. When  $\Omega > \Omega_{opt}$ , the polaron effect is relatively weak, and therefore reducing  $\Omega$  in this regime enhances superconductivity. When  $\Omega < \Omega_{opt}$ , the polaron effect starts to dominate over superconductivity, and therefore further reducing  $\Omega$  suppresses superconductivity. Introducing the Hubbard  $U$  suppresses *both* superconducting and polaron effects, but it suppresses the dominant effect more efficiently: For  $\Omega > \Omega_{opt}$ , it mainly suppresses the superconducting effect; for  $\Omega < \Omega_{opt}$ , it mainly suppresses the polaron effect, and therefore enhances superconductivity. To make this statement more quantitative, in Table I we provide the corresponding  $Z$  and  $\phi$  of the superconducting gap for these two representative  $\Omega$  at  $U = 0$  to  $0.6$ . For  $\Omega = 0.50$ , where superconductivity dominates at  $U = 0$ , both  $Z$  and  $\phi$  are reduced upon increasing  $U$ , with  $\phi$  decreasing faster [see the upper half of Table I]. Accordingly, the resulting gap monotonously decreases upon increasing  $U$ . For  $\Omega = 0.37$ , where the polaron effect dominates at  $U = 0$ , the reductions of  $Z$  and  $\phi$  are more complicated. When  $U \lesssim 0.4$ ,  $Z$  decreases faster than  $\phi$ , and the resulting gap increases upon increasing  $U$ . When  $U > 0.4$ ,  $Z$  decreases slower than  $\phi$ , and the resulting gap increases upon increasing  $U$  [see the lower half of Table I]. In other words, the non-monotonous behavior for  $\Delta(U)$  in the  $\Omega < \Omega_{opt}$  regime originates from the different decreasing rates of the superconducting and polaron phases.

Fig. 2 gives the spectral functions for these two representative  $\Omega$  at  $U = 0, 0.2, 0.4$ , and  $0.6$ . As the Hubbard  $U$

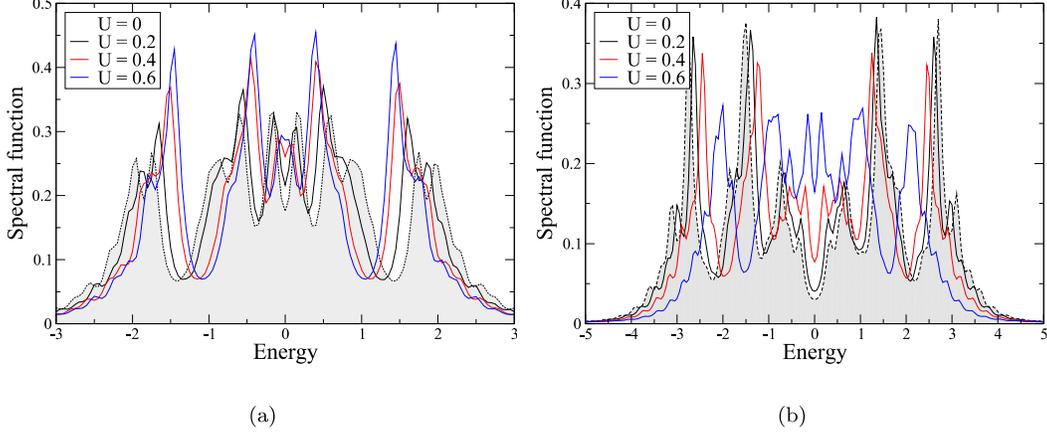


FIG. 2: The spectral functions for  $g = 0.6$  and half filling, with several values of Hubbard  $U = 0, 0.2, 0.4, 0.6$ . As the reference, the dashed curves with shaded area represent  $U = 0$  results. The reduction in the spectral function around zero can originate from superconductivity and polaron effect. (a) For  $\Omega = 0.5$  ( $> \Omega_{opt}$ ), the polaron effect is weak; as  $U$  increases, the spectral function around zero increases, indicates the suppression of superconductivity. (b) For  $\Omega = 0.37$  ( $< \Omega_{opt}$ ), the polaron effect is strong; as  $U$  increases, the spectral function around zero increases, indicates the suppression of polaron effect. For both  $\Omega$  at large  $U$ , the system becomes metallic.

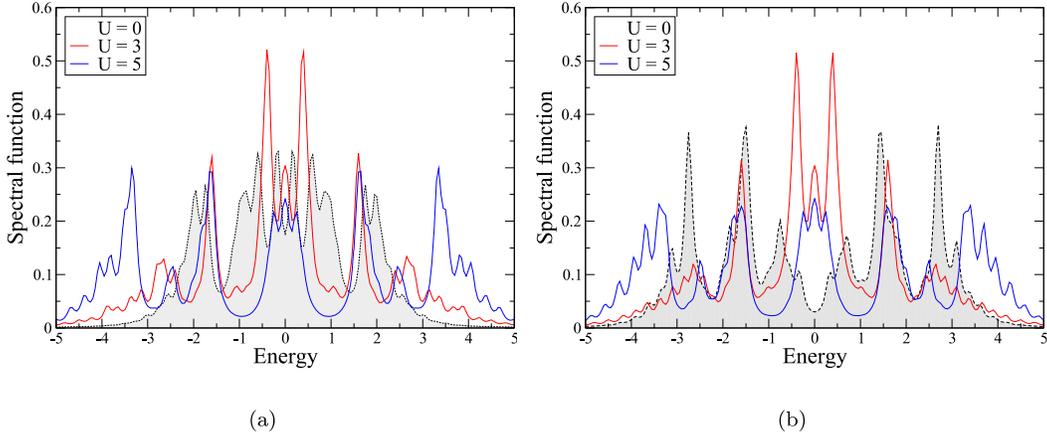


FIG. 3: The spectral functions for  $g = 0.6$  and half filling for two representative (a)  $\Omega = 0.5$  and (b)  $\Omega = 0.37$ , with the Hubbard  $U = 0, 3$ , and  $5$ . As the reference, the dashed curves with shaded area represent  $U = 0$  results. Regardless of  $\Omega$ , upon increasing  $U$  the spectral function around zero first increases, which is a consequence of  $U$  suppressing the polaron effect; further increasing  $U$  reduces the spectral function around zero, which is the precursor of the Mott insulating phase.

suppresses the polaron effect (making  $Z$  smaller) for all  $\Omega$ , the spectral function around zero are expected to increase upon increasing  $U$ . This general behavior is seen for both  $\Omega = 0.5$  [Fig. 2 (a)] and  $\Omega = 0.37$  [Fig. 2 (b)], with the latter more pronounced. This is consistent with the  $Z$  values provided in Table I: For  $U = 0.5$ ,  $Z(U = 0.6)/Z(U = 0)$  value is about 0.72; whereas for  $U = 0.37$ , the reduction of  $Z(U = 0.6)/Z(U = 0)$  value is about 0.10. The Hubbard  $U$  also suppresses superconductivity (making  $\phi$  smaller) for all  $\Omega$ , and this is reflected in the “dip” structure in the spectral function around zero energy. For  $\Omega = 0.5$ , the dip structure becomes less pronounced upon increasing  $U$ , indicating the suppression of superconductivity. For  $\Omega = 0.37$ , the change of the dip structure is more difficult to tell upon increasing  $U$ , as it mixes with the enhancement of  $Z$ . In this regime, we cannot easily distinguish the polaron from the superconducting effect from the spectral functions alone. We need to explicitly compute  $Z$  and  $\phi$  to make the conclusion. To complete the description to the “strongly correlated” limit, in Fig. 3 we show the spectral functions for  $\Omega = 0.5$  and  $\Omega = 0.37$  at  $U = 0, 3$ , and  $5$ . For both  $\Omega$  upon increasing  $U$ , the spectral functions around

zero first increases, which is a consequence of  $U$  suppressing the polaron effect. Further increasing  $U$  reduces the spectral function around zero, which is the precursor of the Mott insulating phase. According to our simulations of intermediate  $U = 5$  [close to the metal-insulator transition, but at metallic side. See last column in Table I], larger effective electron-Boson coupling (smaller  $\Omega$  for a fixed  $g$ ) makes the system more metallic (smaller  $Z$ ), which is consistent with the expectation that electron-phonon coupling generically generates a negative on-site interaction and therefore reduces the effect of Hubbard  $U$  [33, 34, 53].

We now comment on some results in the literature. As we focus on the weak  $U$  limit, we include the results of Holstein model. Within the framework of DMFT, the popular impurity solvers include the Hirsch-Fye [58] Quantum Monte Carlo (QMC) [33, 34], the second order perturbation in phonon propagators [33], the semiclassical solver [30, 32], the path integral [40], the diagrammatic expansion [41], and the continuous time QMC [53]. The continuous time QMC results (which is exact) in Ref. [53] focus on the Mott regime, and in the previous paragraph we show our ED solver leads to the consistent conclusion in this limit. The Hirsch-Fye QMC [33, 34] is formally exact, and works well at high temperature. By computing the corresponding susceptibilities at non-zero temperatures, the charge density wave (CDW) and superconducting  $T_c$  (where the susceptibilities diverge) can be determined. As the ED solver works best for zero-temperature phases, a direct comparison is not possible. However, we notice that the obtained polaron insulating solution, where the local occupation prefers either zero or double electrons, can easily lead to some CDW order. Moreover, by explicitly breaking the symmetry, our ED solver shows that the superconducting state can dominate over the polaron state at larger Boson energy  $\Omega$ . The semiclassical solver [30, 32] neglects the Boson dynamics, and captures only the polaron but not the superconducting physics. The analysis based on path integral [40] and diagrammatic expansion [41] identifies a dimensionless parameter  $\lambda = g^2/(\Omega t)$ , above some critical value (of order one) the system becomes a polaron insulator. Our calculation is consistent with this conclusion, as the superconducting solution can only be stabilized below some critical  $\lambda$  (i.e. at some large enough  $\Omega$  for a fixed  $g$ ), and subtle role of the weak Hubbard  $U$  is present when  $\lambda$  is close to the critical value. There are also algorithms that directly solve the lattice problem, such as the diagrammatic Monte-Carlo [59] and variational Monte-Carlo [60, 61]. These methods typically do not consider the superconducting state, so we do not make further comments on them.

Now we discuss some experimental implications. Our calculation suggests that when the electron-boson coupling is large (measured by  $g^2/\Omega t$ ), where the main effect of boson is to drag the electron motion and to make system more insulating, reducing the electron-boson coupling by *increasing* the local repulsion is actually beneficial to superconductivity. We believe any mechanism that effectively suppresses the electron-boson coupling leads to same effect. A recent experiment shows that shining lights on  $K_3C_{60}$  appears to drastically increase the  $T_c$  from 20 K to 200 K [62], and this strong enhancement is accompanied by the disruption of the competing CDW correlation. Our model calculation provides the following qualitative interpretation. The electron-phonon coupling accounts for both superconducting and CDW correlation in  $K_3C_{60}$ , with the latter being dominant. Shining lights on  $K_3C_{60}$  reduces the electron-phonon coupling, which mainly suppresses the dominant CDW correlation and therefore enhances the superconducting  $T_c$ . Here, the light plays the same role as that of Hubbard  $U$ .

#### IV. CONCLUSION

To conclude, we examine the superconducting solution in the Hubbard-Holstein model, with semicircular electronic DOS at half filling, using Dynamical Mean Field Theory. The main message from our calculations is that, the on-site repulsion is *not* always against the conventional S-wave superconductivity when the Boson degree of freedom is explicitly taken into account. The underlying physics includes the interplay between the superconducting phase, the polaron effect, and the on-site repulsion; a complete picture is provided as follows. The Holstein term alone provides the effective electron-electron attraction that is essential for superconductivity, but at the same time produces the polaron effect that traps electrons and suppresses the superconductivity. A competition between these two mechanisms leads to an optimal Boson energy  $\Omega_{opt}$  for superconductivity. When lowering  $\Omega$  from a large value, the Boson field becomes easier to induce, and therefore both the polaron effect and superconductivity are enhanced, but at different rates. Above  $\Omega_{opt}$ , superconductivity dominates and lowering  $\Omega$  intensifies superconductivity; below  $\Omega_{opt}$ , the polaron effect dominates and lowering  $\Omega$  weakens superconductivity. A weak on-site repulsion, introduced by Hubbard term, reduces both superconductivity and polaron effect, but it reduces the dominant effect at  $U = 0$  more efficiently. Above  $\Omega_{opt}$ , Hubbard  $U$  mainly suppresses superconductivity. Below  $\Omega_{opt}$ , a weak Hubbard  $U$  mainly suppresses the polaron effect and effectively boosts superconductivity. For all  $\Omega$ , further increasing  $U$  suppresses both superconductivity and polaron

effect, the system first becomes metallic and then a Mott insulator. Although the model considered here involves only the local repulsion, any mechanisms that suppress the polaron effect in principle facilitate superconductivity.

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- [1] L. N. Cooper, Phys. Rev. **104**, 1189 (1956), URL <http://link.aps.org/doi/10.1103/PhysRev.104.1189>.
  - [2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **106**, 162 (1957), URL <http://link.aps.org/doi/10.1103/PhysRev.106.162>.
  - [3] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957), URL <http://link.aps.org/doi/10.1103/PhysRev.108.1175>.
  - [4] G. M. Eliashberg, JEPT **11**, 696 (1960).
  - [5] A. B. Migdal, JEPT **7**, 996 (1958).
  - [6] P. Morel and P. W. Anderson, Phys. Rev. **125**, 1263 (1962), URL <http://link.aps.org/doi/10.1103/PhysRev.125.1263>.
  - [7] P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975), URL <http://link.aps.org/doi/10.1103/PhysRevB.12.905>.
  - [8] G. Bergmann and D. Rainer, Z. Phys. **263**, 59 (1973).
  - [9] G. Grimvall, *The electron-phonon interaction in metal* (North-Holland Publishing Company, 1981).
  - [10] P. B. Allen and B. Mitrovic, Solid State Physics **37**, 1 (1983).
  - [11] In the current context, the system is characterized as "weakly correlated" or "strongly correlated" depending on if the electron-electron interaction is weak or strong (at least comparable) with respect to the renormalized electron band energy.
  - [12] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
  - [13] M. Aichhorn, S. Biermann, T. Miyake, A. Georges, and M. Imada, Phys. Rev. B **82**, 064504 (2010), URL <http://link.aps.org/doi/10.1103/PhysRevB.82.064504>.
  - [14] Z. P. Yin, K. Haule, and G. Kotliar, Nat Phys **7**, 294 (2011), URL <http://www.nature.com/nphys/journal/v7/n4/abs/nphys1923.html#supplementary-information>.
  - [15] A. Mann, Nature **475**, 280 (2011).
  - [16] J. G. Bednorz and K. A. Müller, Zeitschrift für Physik B Condensed Matter **64**, 189 (1986), ISSN 1431-584X, URL <http://dx.doi.org/10.1007/BF01303701>.
  - [17] A. Damascelli, Z. Hussain, and Z.-X. Shen, Rev. Mod. Phys. **75**, 473 (2003), URL <http://link.aps.org/doi/10.1103/RevModPhys.75.473>.
  - [18] Y. Kamihara, H. Hiramatsu, M. Hirano, R. Kawamura, H. Yanagi, T. Kamiya, and H. Hosono, JACS **128**, 10012 (2006), <http://dx.doi.org/10.1021/ja063355c>, URL <http://dx.doi.org/10.1021/ja063355c>.
  - [19] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, JACS **130**, 3296 (2008), <http://dx.doi.org/10.1021/ja800073m>, URL <http://dx.doi.org/10.1021/ja800073m>.
  - [20] J.-F. Ge, Z.-L. Liu, C. Liu, C.-L. Gao, D. Qian, Q.-K. Xue, Y. Liu, and J.-F. Jia, Nat Mater (2015).
  - [21] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998), URL <http://link.aps.org/doi/10.1103/RevModPhys.70.1039>.
  - [22] J. A. Hertz, Phys. Rev. B **14**, 1165 (1976), URL <http://link.aps.org/doi/10.1103/PhysRevB.14.1165>.
  - [23] A. J. Millis, Phys. Rev. B **48**, 7183 (1993), URL <http://link.aps.org/doi/10.1103/PhysRevB.48.7183>.
  - [24] S. L. Sondhi, S. M. Girvin, J. P. Carini, and D. Shahar, Rev. Mod. Phys. **69**, 315 (1997), URL <http://link.aps.org/doi/10.1103/RevModPhys.69.315>.
  - [25] H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. **79**, 1015 (2007), URL <http://link.aps.org/doi/10.1103/RevModPhys.79.1015>.
  - [26] W. Qing-Yan, L. Zhi, Z. Wen-Hao, Z. Zuo-Cheng, Z. Jin-Song, L. Wei, D. Hao, O. Yun-Bo, D. Peng, C. Kai, et al., Chin. Phys. Lett. **29**, 037402 (2012), URL <http://stacks.iop.org/0256-307X/29/i=3/a=037402>.
  - [27] J. J. Lee, F. T. Schmitt, R. G. Moore, S. Johnston, Y.-T. Cui, W. Li, M. Yi, Z. K. Liu, M. Hashimoto, Y. Zhang, et al., Nature **515**, 245 (2014).
  - [28] L. Rademaker, Y. Wang, T. Berlijn, and S. Johnston, New Journal of Physics **18**, 022001 (2016), URL <http://stacks.iop.org/1367-2630/18/i=2/a=022001>.
  - [29] T. Holstein, Ann. Phys. **8**, 325 (1959).
  - [30] A. J. Millis, R. Mueller, and B. I. Shraiman, Phys. Rev. B **54**, 5389 (1996), URL <http://link.aps.org/doi/10.1103/PhysRevB.54.5389>.

- [31] S. Okamoto, A. Fuhrmann, A. Comanac, and A. J. Millis, Phys. Rev. B **71**, 235113 (2005), URL <http://link.aps.org/doi/10.1103/PhysRevB.71.235113>.
- [32] C. Lin and A. J. Millis, Phys. Rev. B **79**, 205109 (2009), URL <http://link.aps.org/doi/10.1103/PhysRevB.79.205109>.
- [33] J. K. Freericks and M. Jarrell, Phys. Rev. B **50**, 6939 (1994), URL <http://link.aps.org/doi/10.1103/PhysRevB.50.6939>.
- [34] J. K. Freericks and M. Jarrell, Phys. Rev. Lett. **75**, 2570 (1995), URL <http://link.aps.org/doi/10.1103/PhysRevLett.75.2570>.
- [35] C. Lin, B. Wang, and K. H. Teo, Phys. Rev. B **93**, 224501 (2016), URL <http://link.aps.org/doi/10.1103/PhysRevB.93.224501>.
- [36] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
- [37] G. Kotliar and D. Vollhardt, Physics Today **57** (2004).
- [38] T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).
- [39] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. **83**, 349 (2011), URL <http://link.aps.org/doi/10.1103/RevModPhys.83.349>.
- [40] P. Benedetti and R. Zeyher, Phys. Rev. B **58**, 14320 (1998), URL <http://link.aps.org/doi/10.1103/PhysRevB.58.14320>.
- [41] A. Deppeler and A. J. Millis, Phys. Rev. B **65**, 224301 (2002), URL <http://link.aps.org/doi/10.1103/PhysRevB.65.224301>.
- [42] J. Hubbard, Proc. R. Soc. Lond. A **276**, 238 (1963).
- [43] H. J. Schulz, Phys. Rev. Lett. **64**, 1445 (1990), URL <http://link.aps.org/doi/10.1103/PhysRevLett.64.1445>.
- [44] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992), URL <http://link.aps.org/doi/10.1103/PhysRevLett.69.168>.
- [45] R. Lemański, J. K. Freericks, and G. Banach, Phys. Rev. Lett. **89**, 196403 (2002), URL <http://link.aps.org/doi/10.1103/PhysRevLett.89.196403>.
- [46] C. J. Halboth and W. Metzner, Phys. Rev. Lett. **85**, 5162 (2000), URL <http://link.aps.org/doi/10.1103/PhysRevLett.85.5162>.
- [47] T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. **95**, 237001 (2005), URL <http://link.aps.org/doi/10.1103/PhysRevLett.95.237001>.
- [48] M. J. Rozenberg, X. Y. Zhang, and G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992), URL <http://link.aps.org/doi/10.1103/PhysRevLett.69.1236>.
- [49] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994), URL <http://link.aps.org/doi/10.1103/PhysRevLett.72.1545>.
- [50] G. Wellein and H. Fehske, Phys. Rev. B **56**, 4513 (1997), URL <http://link.aps.org/doi/10.1103/PhysRevB.56.4513>.
- [51] G. Kalosakas, S. Aubry, and G. P. Tsironis, Phys. Rev. B **58**, 3094 (1998), URL <http://link.aps.org/doi/10.1103/PhysRevB.58.3094>.
- [52] D. Meyer, A. C. Hewson, and R. Bulla, Phys. Rev. Lett. **89**, 196401 (2002), URL <http://link.aps.org/doi/10.1103/PhysRevLett.89.196401>.
- [53] P. Werner and A. J. Millis, Phys. Rev. Lett. **99**, 146404 (2007), URL <http://link.aps.org/doi/10.1103/PhysRevLett.99.146404>.
- [54] A. Liebsch and I. Ishida, Journal of Physics: Condensed Matter **24** (2012).
- [55] C. Lin and A. A. Demkov, Phys. Rev. B **88**, 035123 (2013), URL <http://link.aps.org/doi/10.1103/PhysRevB.88.035123>.
- [56] Three Pauli matrices are  $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ,  $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ , and  $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ .
- [57] We note that in Ref. [40],  $\lambda$  is given by  $g^2/(\Omega^2 t)$  because the local electron density is coupled to the local displacement  $x$ , not the field operator  $a^\dagger + a$ . Identifying  $x \sim \frac{1}{\sqrt{2\Omega}}(a^\dagger + a)$  and neglecting the coefficients of one, we get the expression.
- [58] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986), URL <http://link.aps.org/doi/10.1103/PhysRevLett.56.2521>.
- [59] A. S. Mishchenko, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. B **62**, 6317 (2000), URL <http://link.aps.org/doi/10.1103/PhysRevB.62.6317>.
- [60] M. Hohenadler, H. G. Evertz, and W. von der Linden, Phys. Rev. B **69**, 024301 (2004), URL <http://link.aps.org/doi/10.1103/PhysRevB.69.024301>.
- [61] T. Ohgoe and M. Imada, Phys. Rev. B **89**, 195139 (2014), URL <http://link.aps.org/doi/10.1103/PhysRevB.89.195139>.
- [62] M. Mitrano, A. Cantaluppi, D. Nicoletti, S. Kaiser, A. Perucchi, S. Lupi, P. Di Pietro, D. Pontiroli, M. Ricco, S. R. Clark, et al., Nature **530**, 461 (2016).