Quantitative reliability study of the Migdal-Eliashberg theory for strong electron-phonon coupling in superconductors

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We reassess the validity of the Migdal-Eliashberg (ME) theory for coupled electron-phonon systems for large couplings λ. Although model calculations have found that the ME theory breaks down for $\lambda \sim 0.5$, it is routinely applied for $\lambda > 1$ to strong-coupling superconductors. To resolve this discrepancy, it is important to distinguish between *bare* parameters, used as input in models, and *effective* parameters, derived from experiments. We show explicitly that ME gives accurate results for the critical temperature and the spectral gap for large effective λ. This provides quantitative theoretical support for the applicability of the ME theory to strong-coupling conventional superconductors.

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I. INTRODUCTION

The theory of conventional superconductivity, where pairing is mediated by the coupling of electrons to lattice vibrations, is considered as one of the major achievements of the 20th century in condensed-matter physics. It is based on the relatively simple Eliashberg equations,[1] where vertex corrections are neglected. The application of these equations is justified by Migdal's theorem,[2] which states that vertex corrections are proportional to the effective coupling strength λ and the ratio of phonon $\omega_{\rm ph}$ and electronic energy scale W, which usually is of the order of $1/100$ and less.[3,4] The properties of the superconducting state in the Migdal-Eliashberg (ME) theory are then largely determined by λ, $\omega_{\rm ph}$, and a phenomenological parameter for the Coulomb repulsion μ^*. The ME theory is also routinely used as a standard pairing theory for other situations where a bosonic pairing mechanism is analyzed.[5,6]

A number of studies, mainly based on the Holstein model, which go beyond the ME theory, have illustrated that vertex corrections cannot be neglected for large coupling strength even if the ratio $\omega_{\rm ph}/W$ is very small, and that the ME theory becomes inaccurate when[7] λ exceeds a certain value.[8–12] In the adiabatic limit, Benedetti and Zeyher[8] found a breakdown of Migdal's theorem due to the appearance of additional extremal paths in the action for $\lambda \gtrsim 0.4$.[7] Capone and Ciuchi[11] found quantitative deviations of self-consistent ME calculations from dynamical mean-field theory (DMFT) already for intermediate coupling strengths and qualitatively different behavior for stronger coupling. Alexandrov[9] argued that even in the adiabatic limit, the ME theory breaks down due to bipolaron formation and symmetry breaking when λ exceeds one. For strong-coupling superconductors, values of λ of the order of 1–3 are commonly quoted.[3,4] The model calculations, therefore, suggest that strong-coupling superconductors do not lie within the range of applicability of the ME theory.

The purpose of this paper is to bring the results from the model studies in a form in which they can be compared in a meaningful way to the standard diagrammatic approach for superconductivity. This allows us to clarify the quantitative reliability of the ME theory for relevant values of λ and $\omega_{\rm ph}/W$. If phonon renormalization occurs, it is necessary to distinguish the *bare* model parameters from the *effective* parameters describing the phonon properties.[13–15] The latter correspond to the ones derived from experiment or density functional calculations. We study the Holstein model in the limit where the lattice has infinite dimensions. In this limit, the DMFT[16] becomes exact. These DMFT results serve as a benchmark for ME calculations.

We show, in qualitative agreement with earlier work in the normal phase,[11] that self-consistent ME calculations become inaccurate already at moderate *bare* coupling, both for electronic and phonon properties. However, in contrast with previous interpretations, we show that at these bare couplings, the effective coupling is very large, i.e., larger than for strong-coupling superconductors. For effective couplings relevant for strong-coupling superconductors, the ME theory is still accurate.

In many applications of the ME theory, the phonons are not calculated self-consistently, but taken as an input either from a different calculation or experiment. Then one is interested in how accurately electronic properties are described by the ME equations for a given phonon spectrum. We can check this explicitly by taking DMFT as a benchmark for electronic properties and providing the full phonon spectrum as an input for the ME calculations (termed ME + ph later). We show that the electronic properties are predicted very reliably up to large *effective* coupling strengths within ME + ph calculations, i.e., with an accuracy of better than 10%. In this paper, we will neglect the effect of the Coulomb interaction usually taken into account via the parameter μ^*.

The paper is structured as follows: In Sec. II, we first recall the usual definition of the pairing function $\alpha^2F(\omega)$ and the coupling strength λ. Then we give explicit details for the DMFT and ME approaches. In Sec. III, results for the comparison of the DMFT and ME calculations are shown, followed by the conclusions in Sec. IV.

II. MODEL AND FORMALISM

A. Pairing function

The pairing function $\alpha^2F(\omega)$ is an essential ingredient for conventional superconductivity. It can be defined by[3,4]

$$\alpha^2_{\boldsymbol{k},\boldsymbol{k}'}F(\omega) = \rho_0|g_{\boldsymbol{k},\boldsymbol{k}'}|^2\rho^D_{\boldsymbol{k}-\boldsymbol{k}'}(\omega), \tag{1}$$

where ρ_0 is the electronic density of states at the Fermi level, $g_{\boldsymbol{k},\boldsymbol{k}'}$ is the electron-phonon coupling matrix element, and $\rho^D_{\boldsymbol{q}}(\omega)$ is the phonon spectral function, related to the phonon propagator as

$$D_{\boldsymbol{q}}(i\omega_m) = \int_0^\infty d\omega\ \rho^D_{\boldsymbol{q}}(\omega)\frac{2\omega}{(i\omega_m)^2-\omega^2}. \tag{2}$$

These are the dressed phonon quantities of the interacting system. In conventional theory, these are often taken from experiment or estimated by a different method, and then inserted in the Eliashberg equations to solve for T_c, the spectral gap, and other properties. As the properties of conventional superconductivity are mostly confined to a small window around the Fermi energy, often a Fermi-surface average is used,

$$\alpha^2F(\omega) = \frac{1}{\rho_0^2}\sum_{\boldsymbol{k},\boldsymbol{k}'}\alpha^2_{\boldsymbol{k},\boldsymbol{k}'}F(\omega)\delta(\varepsilon_{\boldsymbol{k}}-\mu)\delta(\varepsilon_{\boldsymbol{k}'}-\mu). \tag{3}$$

Then the superconducting state is largely determined through the coupling constant[4,17,18] λ,

$$\lambda = 2\int_0^\infty d\omega\ \frac{\alpha^2F(\omega)}{\omega}. \tag{4}$$

B. Holstein model and DMFT approach

Our quantitative test of the ME theory is based on a model that has been frequently used in the literature, the Holstein model:

$$H = -\sum_{i,j,\sigma}(t_{ij}c^\dagger_{i,\sigma}c_{j,\sigma}+\text{H.c.}) + \omega_0\sum_i b^\dagger_i b_i + g\sum_i(b_i+b^\dagger_i)\left(\sum_\sigma \hat{n}_{i,\sigma}-1\right). \tag{5}$$

Here, $c^\dagger_{i,\sigma}$ creates an electron at lattice site i with spin σ, $b^\dagger_i$ creates a phonon with oscillator frequency ω_0, and $\hat{n}_{i,\sigma} = c^\dagger_{i,\sigma}c_{i,\sigma}$. The electronic density is coupled to an optical phonon mode with coupling constant g. We have set the ionic mass to $M = 1$ in (5). The local oscillator displacement is related to the bosonic operators by $\hat{x}_i = (b_i + b^\dagger_i)/\sqrt{2\omega_0}$, where $\hbar = 1$.

For the DMFT at $T = 0$, we solve the effective impurity problem with the numerical renormalization group[19,20] (NRG) adapted to the case with symmetry breaking.[21,22] The logarithmic discretization parameter is $\Lambda = 1.8$, and we keep about 1000 states at each iteration. The initial bosonic Hilbert space is restricted to a maximum of 50 states. We use a semi-elliptic density of states (DOS) for the electrons, $\rho_0(\varepsilon) = \sqrt{4t^2-\varepsilon^2}/(2\pi t^2)$, with bandwidth $W = 4t$. In terms of the Hilbert transform $\mathrm{HT}[\rho_0](z)$ we have, for the diagonal Green's function,

$$G_{11}(i\omega_n) = A_G\mathrm{HT}[\rho_0](\varepsilon_+) + B_G\mathrm{HT}[\rho_0](\varepsilon_-), \tag{6}$$

and for the off-diagonal part,

$$G_{21}(i\omega_n) = A_F\mathrm{HT}[\rho_0](\varepsilon_+) + B_F\mathrm{HT}[\rho_0](\varepsilon_-). \tag{7}$$

We have defined $A_G = [\zeta_2(i\omega_n)+\varepsilon_+(i\omega_n)]/[\varepsilon_+(i\omega_n)-\varepsilon_-(i\omega_n)]$, $B_G = [\zeta_2(i\omega_n)+\varepsilon_-(i\omega_n)]/[\varepsilon_-(i\omega_n)-\varepsilon_+(i\omega_n)]$, $A_F = \Sigma_{21}(i\omega_n)/[\varepsilon_+(i\omega_n)-\varepsilon_-(i\omega_n)]$, and $B_F = \Sigma_{21}(i\omega_n)/[\varepsilon_-(i\omega_n)-\varepsilon_+(i\omega_n)]$, where

$$\varepsilon_\pm = \frac{\zeta_1(i\omega_n)-\zeta_2(i\omega_n)}{2} \pm \frac{1}{2}\sqrt{[\zeta_1(i\omega_n)+\zeta_2(i\omega_n)]^2 - 4\Sigma_{21}(i\omega_n)\Sigma_{12}(i\omega_n)}, \tag{8}$$

with $\zeta_1(z) = z+\mu-\Sigma_{11}(z)$ and $\zeta_2(z) = z-\mu-\Sigma_{22}(z)$. For the Nambu Green's functions, we have $G_{12}(i\omega_n) = G_{21}(i\omega_n)$ and $G_{22}(i\omega_n) = -G_{11}(-i\omega_n)$. This implies that $\Sigma_{12}(i\omega_n) = \Sigma_{21}(i\omega_n)$ and $\Sigma_{22}(i\omega_n) = -\Sigma_{11}(-i\omega_n)$ for the self-energies. At half filling, $G_{11}(i\omega_n)$ and $\Sigma_{11}(i\omega_n)$ are imaginary functions, whereas $G_{21}(i\omega_n)$ and $\Sigma_{21}(i\omega_n)$, and $D(i\omega_m)$ and $\Sigma_{\mathrm{ph}}(i\omega_m)$, are real functions. For the semi-elliptic DOS, the Hilbert transform is given by

$$\mathrm{HT}[\rho_0](z) = \int_{-D}^{D}d\varepsilon\ \frac{\rho_0(\varepsilon)}{z-\varepsilon} = \frac{1}{2t^2}\left\{z-\mathrm{sgn}[\mathrm{Im}(z)]\sqrt{z^2-4t^2}\right\}, \tag{9}$$

where the square root of a complex number w is given by $\sqrt{r}e^{i\varphi/2}$, where $\varphi = [0,2\pi)$, such that the imaginary part of $\sqrt{w}$ is positive.

At finite temperature, we use the continuous-time quantum Monte Carlo (QMC) method developed for electron-phonon systems.[23] To calculate T_c, we study the susceptibility in the pairing channel, $\chi(\boldsymbol{q},i\omega_n)$, in the limit $\boldsymbol{q}\to 0$ and $i\omega_n\to 0$. It can be expressed in terms of the irreducible vertex in the particle-particle channel $\Gamma^{(\mathrm{pp})}$, which is calculated in the QMC procedure.[16] It is then sufficient to analyze when the largest eigenvalue of the symmetric matrix,

$$M_{n_1,n_2} = \frac{1}{\beta}\sqrt{\tilde{\chi}^0(i\omega_{n_1})}\left[\Gamma^{(\mathrm{pp})}(i\omega_{n_1},i\omega_{n_2};0)\right]\sqrt{\tilde{\chi}^0(i\omega_{n_2})}, \tag{10}$$

exceeds one. We have defined the pair propagator[16]

$$\tilde{\chi}^0(i\omega_{n_1}) = \frac{G(i\omega_{n_1})-G(-i\omega_{n_1})}{\zeta(-i\omega_{n_1})-\zeta(i\omega_{n_1})}, \tag{11}$$

$\zeta(i\omega_n) = i\omega_n+\mu-\Sigma(i\omega_n)$, where $G(i\omega_{n_1})$ is the local lattice Green's function in the normal state.

C. ME approach

The matrix equation for the electronic self-energies in the ME theory (see Fig. 1) reads

$$\underline{\Sigma}(i\omega_n) = -\frac{1}{\beta}\sum_m g^2\tau_3\underline{G}(i\omega_m+i\omega_n)\tau_3D(i\omega_m), \tag{12}$$

where

$$\underline{G}_{\boldsymbol{k}}(i\omega_n)^{-1} = \underline{G}^0_{\boldsymbol{k}}(i\omega_n)^{-1} - \underline{\Sigma}(i\omega_n), \tag{13}$$

with $G_{ij}(i\omega_n) = \sum_{\boldsymbol{k}}G_{ij,\boldsymbol{k}}(i\omega_n)$ and $\underline{G}^0_{\boldsymbol{k}}(i\omega_n)^{-1} = i\omega_n - \tau_3(\varepsilon_{\boldsymbol{k}}-\mu)$. Notice that we use the form valid for a large coordination number, such that only local lattice Green's functions enter. These are calculated with the same semi-elliptic DOS as in Eqs. (6) and (7) for the DMFT calculation. Thus, by ME theory, we mean the diagrammatic theory, which

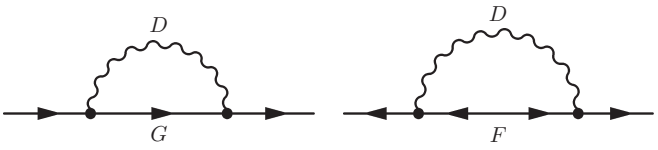

FIG. 1. Diagrams for diagonal and off-diagonal self-energy in the ME theory involving the full electronic Green's function G, anomalous part F, and full phonon propagator D.

neglects all vertex corrections to (12), and this is compared to the full DMFT results. No further approximations, such as assuming a constant density of states or large bandwidth, are made. The latter are common approximations in the literature on the ME theory,[3,4] whose accuracy can be analyzed in an expansion in $\omega_{\rm ph}/W$. This is, however, not the subject of the present paper, where we focus entirely on the accuracy of the theory when vertex corrections are neglected.

The pairing function reads $\alpha^2F(\omega) = \rho_0 g^2 \rho^D(\omega)$ for the Holstein model. In the noninteracting limit, we have $\rho_0^D(\omega) = \delta(\omega-\omega_0) - \delta(\omega+\omega_0)$, which in Eq. (4) gives $\lambda_0 = \rho_0 2g^2/\omega_0$ purely in terms of bare parameters. This quantity was used in model studies and denoted by λ.[7] However, λ as defined in Eq. (4) is given for the *interacting* system.[13–15] Then the phonons are renormalized via the self-energy $\Sigma_{\rm ph}(i\omega_m)$,

$$D(i\omega_m)^{-1} = D^0(i\omega_m)^{-1} - \Sigma_{\rm ph}(i\omega_m), \tag{14}$$

where $D^0(i\omega_m) = 2\omega_0/[(i\omega_m)^2 - \omega_0^2]$. The lowest-order contribution to the phonon self-energy is

$$\Sigma_{\rm ph}(i\omega_m) = \frac{2g^2}{\beta}\sum_n G(i\omega_n)G(i\omega_m + i\omega_n). \tag{15}$$

In the superconducting state there is an additional contribution to $\Sigma_{\rm ph}$ from the off-diagonal Green's function, which is however small and will be neglected in the following. As in Ref. 11, we will call Eqs. (15) and (12) the *self-consistent* ME approximation.

We define the peak of the interacting phonon spectral function $\rho^D(\omega)$ as the effective phonon scale $\omega_{\rm ph} = \omega_0^r$. There is then a mapping of the bare dimensionless parameters $\lambda_0, \omega_0/t$ to the effective parameters $\lambda, \omega_0^r/t$. λ exceeds the bare λ_0 due to the phonon renormalization, $\omega_0 \to \omega_0^r$, and due to the increased lattice fluctuations as shown in the identity valid at $T = 0$,

$$w_D = \int_0^\infty d\omega\ \rho^D(\omega) = 2\omega_0\langle\hat{x}^2\rangle, \tag{16}$$

which is generally larger than one. For a sharply peaked phonon spectrum, the first moment sum rule

$$\int_{-\infty}^{\infty} d\omega\ \omega\rho_D(\omega) = 2\omega_0 \tag{17}$$

implies $w_D \simeq \omega_0/\omega_0^r$. From an estimate for the phonon softening due to the lowest-order diagram, $\omega_0^r/\omega_0 = \sqrt{1-a\lambda_0}$, and Eq. (4), one can then obtain the result $\lambda = \lambda_0/(1-a\lambda_0)$.[2,13,15] In three dimensions, $a = 2$, and for a semi-elliptic DOS in the limit of large dimensions, we have $a = 8/3$.

In order to calculate the gap at $T = 0$, we solve Eq. (12) both by introducing spectral functions and analytic continuation to the real axis, and for comparison directly on the imaginary axis. $D(i\omega_m)$ can be calculated self-consistently via Eq. (15) or taken as an input from DMFT calculations. The latter type of calculation is termed ME + ph. In the ME theory, T_c is calculated by first finding the local lattice Green's function $G(i\omega_n)$ in the normal phase using

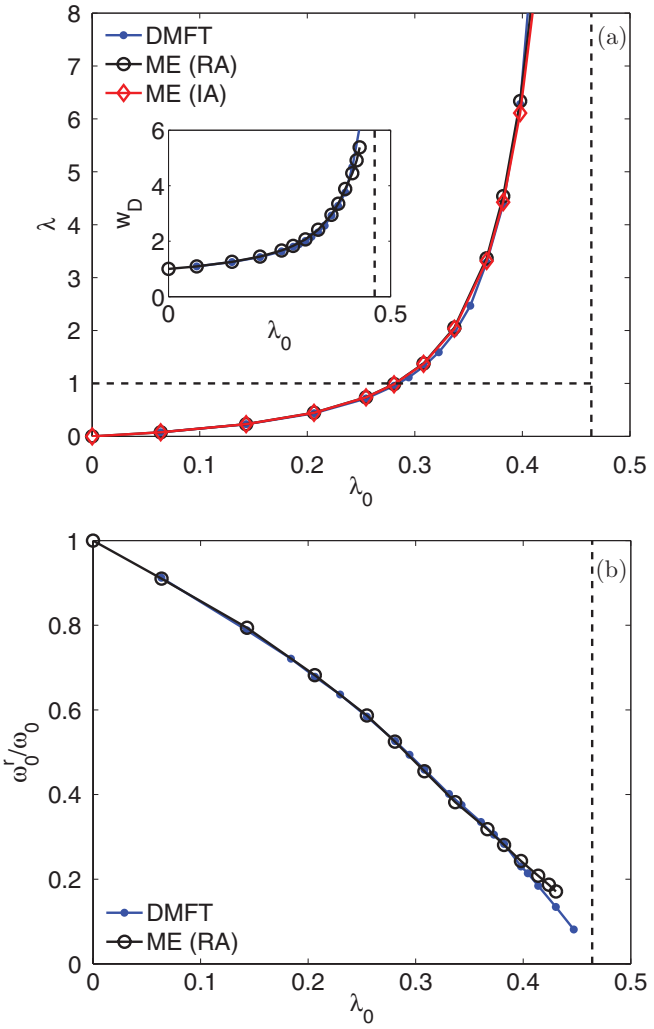

FIG. 2. (Color online) Comparison of the self-consistent ME and DMFT results for renormalized quantities as a function of the bare λ_0: (a) The effective coupling λ as defined by Eq. (4); inset w_D as given by Eq. (16). (b) The ratio of renormalized and bare phonon frequency ω_0^r/ω_0.

$$\Sigma(i\omega_n) = -\frac{g^2}{\beta}\sum_m G(i\omega_m + i\omega_n)D(i\omega_m), \tag{18}$$

and then employing Eq. (10) with

$$\Gamma^{(\rm pp)}\big(i\omega_{n_1}, i\omega_{n_2}; 0\big) = -g^2 D\big(i\omega_{n_1} - i\omega_{n_2}\big). \tag{19}$$

III. RESULTS

Let us first of all establish how the bare and effective quantities are related at $T = 0$. At half filling for fixed $\omega_0 = 0.1t$, we plot λ in Fig. 2(a) and ω_0^r/ω_0 in Fig. 2(b), both as a function of λ_0. We show the results from the self-consistent

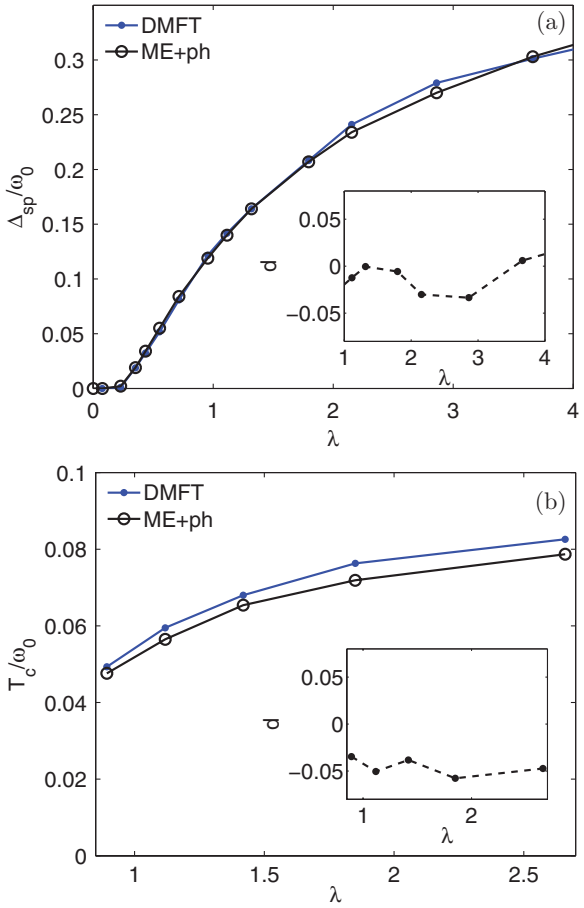

FIG. 3. (Color online) Comparison of quantities for the superconducting state as a function of λ obtained from DMFT and ME calculations with phonon input from DMFT (ME + ph): (a) The spectral gap Δ_{sp}; the inset shows the relative deviation d. (b) The critical temperature for the onset of superconductivity T_c.

ME theory on the real axis (RA) and on the imaginary axis (IA) in comparison with the full DMFT-NRG result.

Here, λ increases slowly for $\lambda_0 \leqslant 0.3$ up to values around one. Then it rises more rapidly close to values of λ_0, where in the normal state a metal-to-bipolaronic (BP) insulator transition had been found at $\lambda_0^c \simeq 0.464$ (shown as a vertical line).[8,10] The behavior is qualitatively similar to the analytic estimate above, however, as $\lambda_0^c > 1/a$, the latter is a substantial overestimate and diverges too quickly. The region of most interest for our purpose is $\lambda \sim$ 1–3, which are typical values for strong-coupling superconductors. This corresponds to $\lambda_0 \sim$ 0.3–0.37 in terms of bare parameters. The values for λ obtained in the self-consistent ME theory compare well to the DMFT results for smaller values of $\lambda_0 \leqslant 0.3$, and then start to overestimate this quantity slightly. For values of λ_0 closer to the BP transition, self-consistent ME underestimates λ. We also compare the effective phonon frequency, which decreases with λ_0 toward zero when λ_0 approaches λ_0^c. This quantity compares well to the DMFT result for a considerable range of λ_0, but starts to deviate for $\lambda_0 > 0.38$ or $\lambda \gtrsim 4$.

We can also calculate electronic properties such as the quasiparticle weight z or the off-diagonal self-energy $\Sigma^{\rm off}(0)$, which roughly determines the spectral gap at zero temperature,

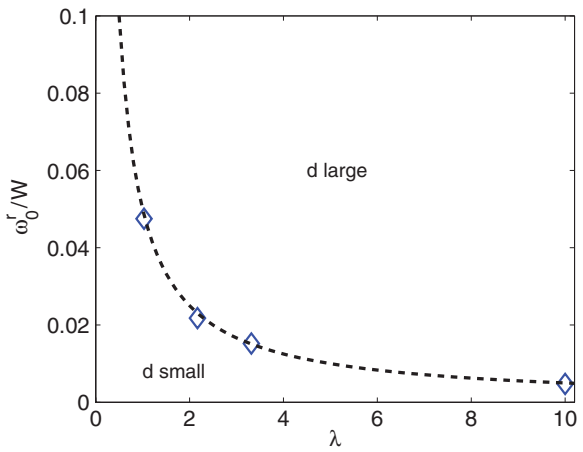

FIG. 4. (Color online) Guideline for the quantitative reliability of the ME theory. The diagram shows points (diamonds) in the ω_0^r/W-λ plane, where the deviation d between the DMFT and ME + ph theory is $d \simeq 0.1$. The dashed line is given by the functional form $\omega_0^r/W = c/\lambda$, which follows from an analytical estimate where the vertex correction exceeds a certain value. $c = 0.05$ was used.

$\Delta_{sp} \simeq z\Sigma^{\rm off}(0)$. Then one finds good agreement for small coupling and moderate deviations between DMFT and self-consistent ME theory in the intermediate coupling regime, and close to the bipolaronic transition, similar to the results for z and ω_0^r that have been obtained by Ciuchi and Capone[11] in the normal state.

Our main objective is to test the validity of the ME theory at strong coupling. Hence, we compare the results for the superconducting properties Δ_{sp} and T_c obtained from the ME + ph calculations with the full DMFT results. In Fig. 3(a), we show Δ_{sp} as extracted from the spectral function computed from ME + ph calculations on the real axis and the corresponding DMFT result. Notice that the results are plotted as a function of λ now.

We find very good agreement for small values of $\lambda < 1$, then a regime where ME + ph slightly underestimates the value for the gap, before it exceeds the DMFT result for larger values of λ. By inspecting the relative deviation $d = (\Delta_{sp}^{ME} - \Delta_{sp}^{DMFT})/\Delta_{sp}^{ME}$, plotted as an inset, we see that there is an agreement in the regime $\lambda \sim$ 1–3 that is better than 10%. At very large values of λ, Δ_{sp} from ME + ph increases more strongly than the DMFT result. For similar parameters, we have also calculated the critical temperature T_c as deduced from the Bethe-Salpeter equation of the uniform pair susceptibility.[24] The comparison of the ME theory and DMFT-QMC result is shown in Fig. 3(b). Good agreement is found in the relevant range for λ. DMFT-QMC systematically slightly underestimates the phonon renormalization, which accounts partly for the discrepancy of T_c from the ME + ph calculations. In a related approach, Marsiglio found, for a 4×4 cluster, that the self-consistent ME theory agrees well with QMC calculations for the pairing susceptibility.[14]

By doing similar comparisons for different bare parameters, we mapped out for which values of the effective parameters λ and ω_0^r/W DMFT and ME + ph show good agreement, i.e., $d \lesssim 0.1$. The results are shown in Fig. 4 and can be well understood in terms of the effective expansion parameter of

the ME theory, $\lambda\omega_0^r/W$, which should not exceed 0.05 for good accuracy. The results can serve as a guideline for the application of the ME theory with reliable phonon input.

IV. CONCLUSIONS

We have assessed the validity of the ME theory. We calculated accurately the effective coupling strength λ in terms of the bare coupling strength λ_0. For intermediate λ_0, the system is close to a bipolaronic metal-insulator transition and λ is very strongly enhanced. Close to this point, the ME theory breaks down. However, for typical values for strong-coupling superconductors, $\lambda \sim 1$–3, the ME theory is very accurate for small values of $\omega_{\rm ph}/W$. This result is demonstrated explicitly for the Holstein model in the limit of large dimensions, where most of the spectral weight of the pairing function is located at $\omega_{\rm ph}$. We expect that this result is also applicable for more general forms of pairing functions, $\alpha^2F(\omega)$, in three dimensions with an appropriate cutoff scale $\omega_{\rm ph}$. In many applications of the ME theory, a momentum average over the Fermi surface is taken, such that the situation is similar to the one studied here. However, the momentum dependence can be important in certain cases, especially for lower dimensional materials. For instance, in Ref. 25, the momentum dependence of vertex corrections and their effect on T_c were analyzed.

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