Accuracy of Migdal-Eliashberg theory and Coulomb pseudopotential

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The Migdal-Eliashberg (ME) theory provides a very successful method for describing conventional superconductors, where the pairing is driven by a phonon-induced attraction. This theory is based on Migdal's theorem, stating that vertex corrections can be neglected if the phonon energy scale (ω_0) is much smaller than the electronic energy scale (D). This should be true even if the dimensionless effective electron-phonon coupling λ is much larger than unity, as long as $(\omega_0/D)\lambda \ll 1$. Thus vertex corrections are neglected in ME theory, which is a huge simplification.

An important issue for conventional superconductors is why the weak phonon-induced attraction can drive superconductivity in spite of the large Coulomb repulsion. Morel and Anderson [1] and others showed that retardation effects play an important role. Due to the very different energy scales for electrons and phonons, the destructive effects of the Coulomb interaction on superconductivity can be dramatically reduced. This is included in ME theory as a strongly reduced Coulomb pseudo potential [1]

$$\mu^* = \frac{\mu}{1+\mu \log(D/\omega_0)}, \tag{1}$$

where $\mu = \rho_0 U$, U is a typical Coulomb interaction, ρ_0 is the density of states at the Fermi energy and D is half the band width. Since $\omega_0 \ll D$, μ^* can be small even if μ is very large.

In spite of the huge success of ME theory questions have been raised about its validity. Several groups have peformed accurate calculations for the Holstein model. From these calculations it was concluded that ME theory may break down already for small values of $\lambda \sim 1/2$, even if ω_0/D is very small. ME theory would then not apply to strong-coupling superconductors with $\lambda \sim 1-3$. Below we reconsider these results for the Holstein model used in earlier approaches.

The electron-phonon interaction is expected to be treated very accurately in ME theory, thanks to Migdal's theorem. The treatment of the Coulomb interaction is much harder, due to the absence of a theorem equivalent to Migdal's theorem. Morel and Anderson treated the Coulomb interaction in a similar way as the electron-phonon interaction is treated in ME theory, although the neglect of vertex corrections for the Coulomb interaction is questionable. For instance, we have studied the retardation effects due to higher subbands in alkali-doped fullerides [2]. Following the Morel and Anderson approach we found that the higher sub bands greatly reduce μ^*. This is an unphysical result, and it is due to the neglect of vertex corrections [2]. Below we consider the renormalization of μ^* for the Hubbard-Holstein model.

The effective electron-phonon coupling strength λ [3] is of crucial importance for the understanding of the accuracy of ME. It is defined as

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

where the pairing function $\alpha^2 F(\omega)$ is defined

$$\alpha^2 F(\omega) = \frac{1}{\rho_0}\sum_{\mathbf{k}\mathbf{k}'} |g_{\mathbf{k}\mathbf{k}'}|^2 \rho^{\rm ph}_{\mathbf{k}-\mathbf{k}'}(\omega)\delta(\mu-\varepsilon_{\mathbf{k}})\delta(\mu-\varepsilon_{\mathbf{k}'}), \tag{3}$$

in terms of the electron-phonon coupling constants $g_{\mathbf{k}\mathbf{k}'}$ and the phonon spectral function $\rho^{\rm ph}_{\mathbf{q}}(\omega)$ for the wave vector $\mathbf{q}$. Here, $\varepsilon_{\mathbf{k}}$ is the energy of an electronic state with the wave vector $\mathbf{k}$ and μ is the chemical potential. We also define a bare coupling, λ_0, which is obtained from Eq. (2) if the spectral function $\rho^{\rm ph}_{\mathbf{q}}(\omega)$ is replaced by results for noninteracting phonons. The effective λ is typically larger than the bare λ_0, due to a renormalization of $F(\omega)$ and the effective phonon frequency ω_0^r [3].

We first study the accuracy of ME theory, neglecting the Coulomb interaction [4]. We address the Holstein model, using the dynamical mean-field theory (DMFT). We consider the model for infinite dimension, where DMFT becomes exact. The results are compared with ME theory. We use a semielliptical electron density of states with the band width $2D$ and the bare phonon frequency $\omega_0 = 0.05D$.

Fig. 1 shows λ as a function of λ_0 for the Holstein model. The figure illustrates how λ grows much faster than λ_0 for $\lambda_0 \gtrsim 0.3$. The rapid increase in λ is partly due to the spectral weight $\rho^{\rm ph}_{\mathbf{q}}(\omega)$ being shifted to lower

energies, lowering ω_0^r. Due to the ω in the denominator of Eq. (2) this increases λ. A second contribution is the normalization w_D of $\rho_{\mathbf{q}}^{\rm ph}(\omega)$, which increases approximately as $1/\omega_0^r$. For $\lambda_0 = 0.464$ (shown by a vertical dashed line) there is a transition to bipolaron insulator. Conventional superconductors therefore correspond to parameters in the range $\lambda_0 < 0.464$. This range contains values for the effective $\lambda \sim 1 - 3$ observed for strong-coupling superconductors.

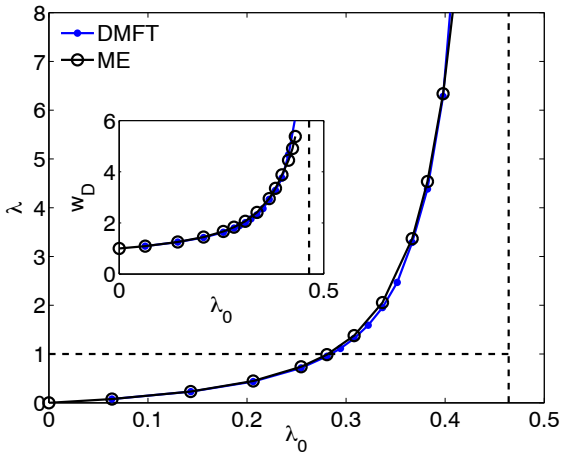

Figure 1: Effective λ as a function of bare λ_0. The inset shows the normalization w_D of the phonon spectral function.

For practical uses of ME theory, the information about the phonons and their coupling to the electrons is typically obtained either from experiment or from density functional calculations. In both cases the input is the effective λ and renormalized phonons. To test the accuracy of ME theory we therefore follow this approach and obtain the phonon information from DMFT. We then calculate the superconductivity gap in ME theory and compare this with exact DMFT results.

Fig. 2 shows the superconductivity gap as a function of the effective λ. ME theory agrees to within a few per cent with DMFT up to the largest values of λ studied. We therefore conclude that ME theory indeed is accurate if the Migdal condition, expressed in effective quantities, $(\omega_0^r/D)\lambda \ll 1$, is fulfilled. In Fig. 2, $(\omega_0^r/D)\lambda \lesssim 0.05$ is much smaller than unity.

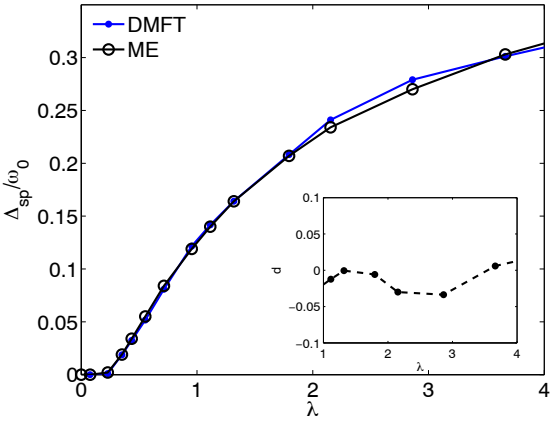

Figure 2: Superconductivity gap as a function of effective λ according to ME theory and DMFT. The inset shows the relative deviation of ME theory.

We now turn to the Coulomb pseudo potential μ^*. To address superconductivity we need to calculate the pairing susceptibility χ. A divergence of χ signals that the system goes superconducting. χ can be expressed in terms of the irreducible vertex Γ as

$$\chi = \chi_0^{1/2}(1 - \chi_0^{1/2}\Gamma\chi_0^{1/2})^{-1}\chi_0^{1/2} \equiv \chi_0^{1/2}A\chi_0^{1/2}, \tag{4}$$

where χ_0 is a noninteracting propagator consisting of a product of two dressed Green's functions. If the vertex is calculated to lowest nontrivial order in the electron-phonon interaction, ME theory is obtained. In a similar way Morel and Anderson [1] studied Γ to lowest order in the Coulomb interaction. To proceed, we can project out higher frequencies from the matrix A and obtain an effective A only containing frequencies smaller than, say, ω_0. This describes the effects of retardation. Considering just the lowest order in U, neglecting the electron-phonon interaction and assuming a constant density of states, we obtain the Morel-Anderson result in Eq. (1). While the

limitation to the lowest order contribution to Γ in λ is justified by Migdal's theorem, this justification does not apply for the Coulomb interaction. We have therefore calculated the vertex to second order in U for the Hubbard model assuming a constant density of states.

Based on the result in Eq. (1), we may guess that μ^* takes the form

$$\mu^* = \frac{\mu + a\mu^2}{1 + \mu\log(\frac{D}{\omega_0}) + a\mu^2\log(\alpha\frac{D}{\omega_0})}. \tag{5}$$

Here $a = \chi_0/\rho_0 = 1.38$ is a prefactor describing the importance of the second order term in the absence of retardation effects. The second order term should also contribute to retardation effects and therefore we have added a new term in the denominator. However, due to a different frequency dependence for the second order term we expect retardation effects to be weaker. This is supposed to be described by $\alpha < 1$.

Calculating Γ up to second order in U leads to terms in μ^* to infinite order. These terms can be calculated analytically up to order U^3. We can then identify terms order by order in Eq. (5) and determine $\alpha = 0.10$. This small factor is a measure of the less efficient retardation effects of the second order contribution. This result together with numerical calculations are shown in Fig. 3. Since the Ansatz by construction is correct to order U^3, it agrees with the numerical calculations up to moderate values of $\mu \sim 0.4$. The second order contribution increases μ^* appreciably. Furthermore, the numerical calculation shows that μ^* does not saturate as μ is increased.

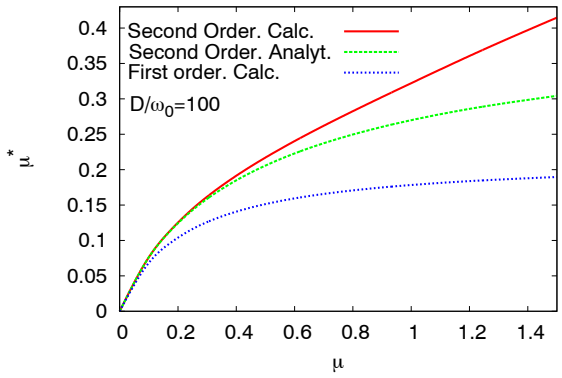

Figure 3: Coulomb pseudo potential μ^* as a function of $\mu = U/D$ according to first and second order calculations as well as the analytical Ansatz in Eq. (5).

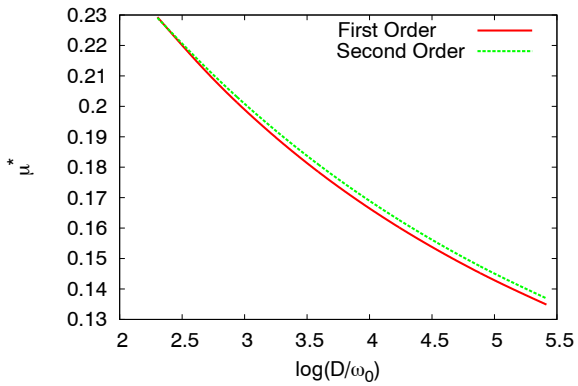

Figure 4: μ_c^* as a function of $\log(D/\omega_0)$ for $\beta\omega_0 = 240$ including first ($\mu_{c1} = 0.5$) or first and second ($\mu_{c2} = 0.2756$) order contributions. μ_{c1} and μ_{c2} were chosen so that the same μ_c^* was obtained in the two calculations for $D/\omega_0 = 10$.

Fig. 4 shows μ^* as a function of D for Γ calculated to first or second order in U. The value of U was adjusted in the two calculations so that μ^* is the same for $D/\omega_0 = 10$. Although the retardation effects are less efficient for the second order contribution, the reduction of μ^* as a function of D is very similar, as can also be derived from Eqs. (1, 5). Similar conclusions can be drawn from a complimentary calculation, where an approximate analytical solution for the pairing equation is derived.

To summarize, the Morel-Anderson theory makes two main predictions: i) as D is increased for fixed U, μ^* goes to zero and ii) as U is increased for fixed D/ω_0, μ^* saturates at the value $1/\log(D/\omega_0)$. Fig. 4 illustrates that i) remains true when the second order contribution is added but Fig. 3 shows that i) is violated, i.e, μ^* does not saturate as U is increased.

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