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Dynamical exchange effects in a two-dimensional many-polaron gas

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Abstract. We calculate the influence of dynamical exchange effects on the response properties and the static properties of a two-dimensional many-polaron gas. These effects are not manifested in the random-phase approximation which is widely used in the analysis of the many-polaron system. Here they are taken into account by using a dielectric function derived in the time-dependent Hartree-Fock formalism. At weak electron-phonon coupling, we find that dynamical exchange effects lead to substantial corrections to the random-phase approximation results for the ground state energy, the effective mass, and the optical conductivity of the polaron system. Furthermore, we show that the reduction of the spectral weight of the optical absorption spectrum at frequencies above the longitudinal optical phonon frequency, due to many-body effects, is overestimated by the random-phase approximation.

PACS. 71.45.Gm Exchange, correlation, dielectric and magnetic response functions, plasmons – 71.10.Pm Fermions in reduced dimensions (anyons, composite fermions, Luttinger liquid, etc.) – 71.38.Fp Large or Fröhlich polarons

1 Introduction

Although the static and dynamic properties of a single polaron have been [1,2] (and still are [3]) extensively studied, the properties of an interacting polaron system, e.g. its optical absorption [4,5], are less well understood. Thus far, the many-polaron system has been studied mainly in the Hartree-Fock approximation and in the random-phase approximation (RPA) [6–9], even though in reference [10] it was shown that in three dimensions (3D) the polaron energy and effective mass are influenced by screening effects beyond RPA. In this paper, we investigate dynamical exchange effects in both static properties (energy and effective mass) and response properties (optical absorption) of the two-dimensional (2D) polaron system.

However, although our formalism is appropriate for the description of an interacting electron (or polaron) gas, it does not allow to investigate the 2D Wigner solid phase formed for example by electrons on a helium surface. Also the study of the many small-polaron gas and bipolarons in quasi-2D systems such as the copper oxide planes in high-T_c cuprate superconductors [11–14] lies beyond the scope of our approach in its current form.

A convenient formalism to take into account many-body effects in the polaron system relies on containing these effects in the structure factor [6]. This approach, reminiscent of the Feynman-Bijl treatment of superfluid helium-4, was first developed to calculate the ground state energy of a many-polaron system [6], and has later been applied to the optical absorption of this system [15]. The 2D dynamic structure factor can be written as

$$S_{2\mathrm{D}}\left(q,\omega\right) = -\frac{\hbar}{n v_q}\,\mathrm{Im}\left(\frac{1}{\varepsilon\left(q,\omega\right)}\right), \tag{1}$$

with $v_q = e^2/(2\varepsilon_\infty q)$ the Fourier transform of the bare Coulomb interaction in 2D, n the surface density of charge carriers, ε_∞ the dielectric constant at high frequency, and $\varepsilon(q,\omega)$ the dielectric function of the system of charge carriers. Previous work [6–9,15] relied on the RPA dielectric function:

$$\varepsilon_{\mathrm{RPA}}(q,\omega) = 1 + Q_0(q,\omega), \tag{2}$$

where $Q_0(q,\omega)$ is the 2D Lindhard polarizability and is known in closed form [16]. A more accurate result for the dielectric function is obtained by introducing the frequency dependent local field correction $G(q,\omega)$:

$$\varepsilon(q,\omega) = 1 + \frac{Q_0(q,\omega)}{1 - G(q,\omega)Q_0(q,\omega)}. \tag{3}$$

In the 3D case, the local field correction was derived in the framework of the dynamical exchange decoupling (DED) method [17]. This method, based on the time-dependent Hartree-Fock formalism, was recently extended to the 2D case in references [18,19]. This leads to an improved dielectric function, $\varepsilon_{\mathrm{DED}}(q,\omega)$, that can be used to include

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dynamical exchange effects in the analysis of the many-polaron system. The DED result for the dielectric function is markedly different from the results obtained in the RPA formalism, Hubbard's formalism [20] and the formalism of Singwi et al. [21]. In 3D these different approaches can be compared to experiment: measurements of the dynamic local field correction by Larson and co-workers [22,23] have shown that the 3D DED approach [17] leads to superior results.

In this work, we use the DED dielectric function in combination with the formalism describing the many-body effects in a polaron system through the structure factor. In Section 2, we investigate the dynamical exchange effects on the optical absorption of the many-polaron system. From the optical conductivity the effective mass of the polaron as a function of the density is derived through a sum-rule in Section 3. Finally, in Section 4, the ground state energy of the interacting polaron system is calculated beyond RPA. As we shall show, including dynamical exchange effects leads to non-negligible corrections to all these quantities.

2 Optical absorption of the interacting 2D polaron system

The optical absorption of an interacting system of Fröhlich polarons in the weak-coupling regime was investigated in [7,15]. The optical conductivity in 2D is given by [15]

$$\mathrm{Re}[\sigma_{2\mathrm{D}}(\omega)] = \alpha \frac{ne^2}{4\omega^3} \int_0^\infty dq\; q^2 S_{2\mathrm{D}}(q, \omega - \omega_{\mathrm{LO}}), \qquad (4)$$

where e is the electron charge, ω_{LO} is the longitudinal optical (LO) phonon frequency and α is the dimensionless Fröhlich coupling constant determining the strength of the electron-phonon interaction. Note that a delta-function peak at $\omega = 0$, omitted in (4), is present in the optical absorption. The influence of the Fermi statistics and the screened Coulomb interactions between the electrons are taken into account through the structure factor $S_{2\mathrm{D}}$ appearing in expression (4). Thus far, the effect of electron-electron interactions on the *optical absorption* of a many-polaron gas has been investigated only in the framework of RPA [4,7,15]. Nevertheless, expression (4) is not restricted to the RPA approximation: any form of the dynamic structure factor can be introduced in the integrand. Here, we will use the results obtained for the dielectric function in the DED formalism [19] instead.

Using expression (1) and the DED result for the dielectric function, we can rewrite (4) as

$$\mathrm{Re}\left[\sigma_{2\mathrm{D}}(\nu)\right] = -\alpha \frac{\mathcal{N}}{(\nu/\nu_{\mathrm{LO}})^3} \times \int_0^\infty dk\; k^3\, \mathrm{Im}\left(\frac{1}{\varepsilon_{\mathrm{DED}}(k, \nu - \nu_{\mathrm{LO}})}\right), \qquad (5)$$

where $k = q/k_F$ and $v = \hbar\omega/(2E_F)$ are dimensionless wave numbers and frequencies based on the Fermi wave vector k_F and the Fermi energy E_F, respectively. The prefactor

$$\mathcal{N} = \frac{n\left(\hbar\omega_{\mathrm{LO}}\right)^2 e^2}{2m_b^2\omega_{\mathrm{LO}}^3} \sqrt{\frac{\hbar}{2m_b\omega_{\mathrm{LO}}}} \frac{4\pi\varepsilon_\infty k_F^2}{e^2} \qquad (6)$$

contains material constants (the band mass m_b, the LO phonon frequency ω_{LO} and the high-frequency permittivity ε_∞) and has dimensions of optical conductivity. Expression (5) for the optical absorption allows to easily substitute available results for the dielectric function.

The DED structure factor can be interpreted as a sum of two contributions, namely a contribution from the single-particle excitations (the Landau continuum) and a contribution from the plasmon excitations. We can write

$$\mathrm{Im}\left[\frac{1}{\varepsilon_{\mathrm{DED}}(k,\nu)}\right] = -A_{\mathrm{pl}}(k)\delta[\nu - \nu_{\mathrm{pl}}(k)] + \mathrm{Im}\left[\frac{1}{\varepsilon_{\mathrm{cont}}(k,\nu)}\right], \qquad (7)$$

where ν_{LO} is the LO phonon frequency in units of $2E_F/\hbar$ and $\nu_{\mathrm{pl}}(k)$ is the plasmon dispersion defined by $\varepsilon(k, \nu_{\mathrm{pl}}) = 0$. The plasmon excitations in our approach lead to delta-functions, with a strength $A_{\mathrm{pl}}(k)$, in the frequency dependence of the structure factor. Also the optical conductivity can be separated in a contribution due to the single-particle excitations and a part coming from the plasmon branch:

$$\mathrm{Re}[\sigma_{2\mathrm{D}}(\nu)] = \mathrm{Re}\left[\sigma_{2\mathrm{D}}^{\mathrm{pl}}(\nu)\right] + \mathrm{Re}\left[\sigma_{2\mathrm{D}}^{\mathrm{cont}}(\nu)\right], \qquad (8)$$

with

$$\mathrm{Re}[\sigma_{2\mathrm{D}}^{\mathrm{pl}}(\nu)] = \alpha \frac{\mathcal{N}}{(\nu/\nu_{\mathrm{LO}})^3} \frac{k_0^3 A_{\mathrm{pl}}(k_0)}{\nu'_{\mathrm{pl}}(k_0)}, \qquad (9)$$

$$\mathrm{Re}[\sigma_{2\mathrm{D}}^{\mathrm{cont}}(\nu)] = -\alpha \frac{\mathcal{N}}{(\nu/\nu_{\mathrm{LO}})^3} \times \int_0^\infty dk\; k^3\, \mathrm{Im}\left(\frac{1}{\varepsilon_{\mathrm{cont}}(k, \nu - \nu_{\mathrm{LO}})}\right). \qquad (10)$$

Here, k_0 is the wave vector at which $\nu - \nu_{\mathrm{LO}} = \nu_{\mathrm{pl}}(k)$, and $\nu'_{\mathrm{pl}} = d\nu_{\mathrm{pl}}/dk$ is the derivative of the plasmon frequency with respect to the wave vector. In the 2D electron gas, the plasmon branch $\nu_{\mathrm{pl}}(k)$ lies close to the edge of the Landau continuum, $k^2/2 + k$. Figure 1 compares the plasmon dispersion in the DED approach to the dispersion in the RPA approach for several values of r_s. For small k values the plasmon frequency in DED is lower than in RPA. Furthermore, in DED longer wave length plasmons are present. The oscillator strength $A_{\mathrm{pl}}(k)$ of the plasmon branch can be obtained straightforwardly using the f-sum rule. If we substitute (7) in the f-sum rule,

$$-\int_0^\infty \nu\, \mathrm{Im}\left(\frac{1}{\varepsilon_{\mathrm{DED}}(k,\nu)}\right) d\nu = \frac{\pi}{2}\frac{r_s k}{\sqrt{2}}, \qquad (11)$$

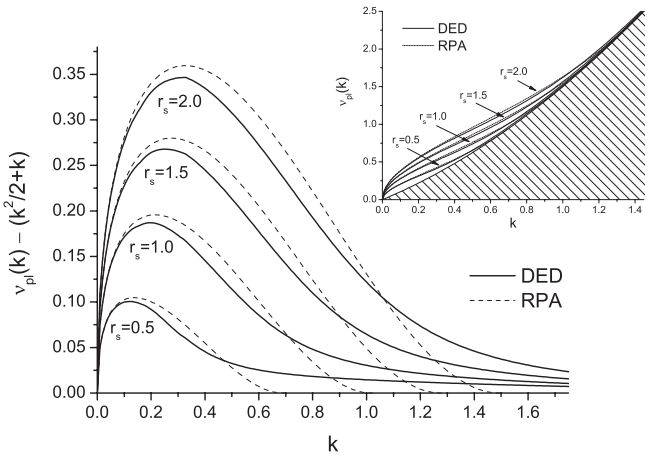

Fig. 1. The plasmon dispersion $\nu_{\rm pl}(k)$ in a 2D electron gas is shown as a function of the wave number k (in units of k_F), relative to the edge of the Landau continuum $k^2/2 + k$, for different values of r_s. The full curves correspond to the DED result, and the dashed curves to the RPA result. In the inset, the location of the plasmon branch and the Landau continuum (hatched area) are shown.

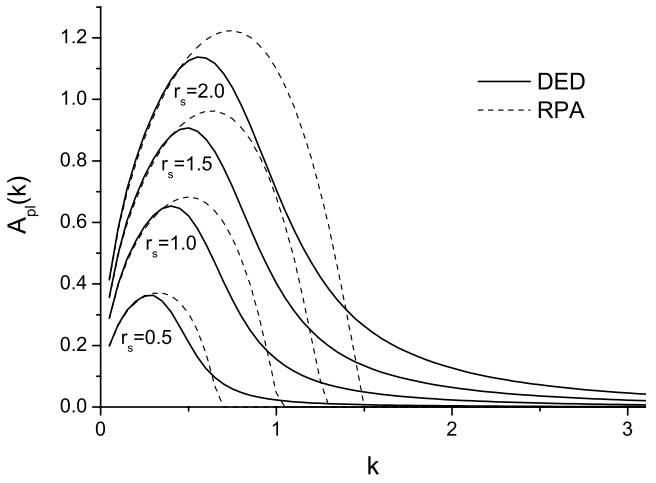

Fig. 2. The oscillator strength $A_{\rm pl}(k)$ of the plasmon excitation in a 2D electron gas at $\nu_{\rm pl}(k)$ is shown as a function of the wave number k (in units of k_F), for different values of r_s. The full curves correspond to the DED result, the dashed curves to the RPA result.

we can find an expression for the oscillator strength of the plasmon branch:

$$A_{\rm pl}(k) = \frac{1}{\nu_{\rm pl}(k)} \left(\frac{\pi}{2} \frac{r_s k}{\sqrt{2}} - M_1 \right), \qquad (12)$$

where

$$M_1 = -\int_0^\infty \nu \, {\rm Im} \left(\frac{1}{\varepsilon_{\rm cont}(k,\nu)} \right) d\nu, \qquad (13)$$

is the first frequency moment of the Landau continuum contribution only. In Figure 2, we compare the oscillator strength of the plasmon branch in RPA and DED for several values of r_s. At small k the difference between the strength of the plasmons in RPA and DED is negligible. As k increases, a difference appears: the maximum oscillator strength for the plasmon branch in DED is reached at a smaller wave vector. Compared to RPA, the oscillator strength of the DED plasmons shows a long tail as a function of k.

In Figure 3 the optical absorption due to the plasmon contribution is shown for several relevant values of the density n of a two dimensional polaron gas, using the material parameters for GaAs ($\varepsilon_\infty = 10.8$, $m_{\rm b} = 0.0657\ m_{\rm e}$, $\hbar\omega_{\rm LO} = 36.77$ meV, $a_{\rm Bohr} = 8.78$ nm). The presence of the shorter wave length plasmons in DED as compared to RPA shifts the spectral weight to higher frequencies. Nevertheless, both in RPA and DED the contribution of plasmons to the optical absorption of the many-polaron gas is small in comparison with the contribution of the single-particle excitations. The total optical absorption is shown in Figure 4, again for different surface densities of polarons in GaAs. Although the Landau continuum occupies the same region of the $\{k, \nu\}$-plane in the DED and RPA approaches, the spectral weight of the structure factor is distributed differently. As can be seen in Figure 4,

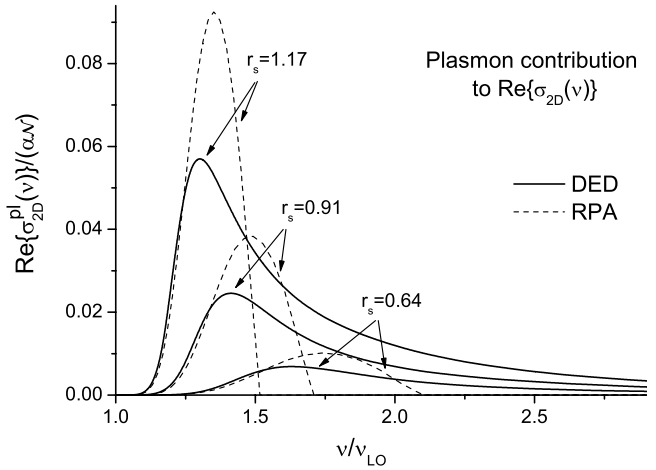

Fig. 3. The contribution of the plasmon excitations to the optical absorption of the many-polaron gas is shown as a function of the frequency ν in units of the LO phonon frequency $\nu_{\rm LO}$, for $r_s = 0.64$ (corresponding to $n = 10^{12}$ cm^{-2}), $r_s = 0.91$ ($n = 5 \times 10^{11}$ cm^{-2}), and $r_s = 1.17$ ($n = 3 \times 10^{11}$ cm^{-2}). Full curves represent the DED result, and dashed curves the RPA result.

this leads to a measurable difference between the DED and RPA results. Comparing both the DED and RPA optical absorption with the single-polaron absorption [24], we find that the RPA result overestimates the damping due to many-body effects.

3 Effective mass of the polaron in DED

From Figure 4, it is clear that the spectral weight of the optical absorption in the region beyond the single-phonon gap ($\omega > \omega_{\rm LO}$) is different for each of the approaches (DED, RPA and single-polaron). This may seem surprising at first glance, since the f-sum rule imposes that the

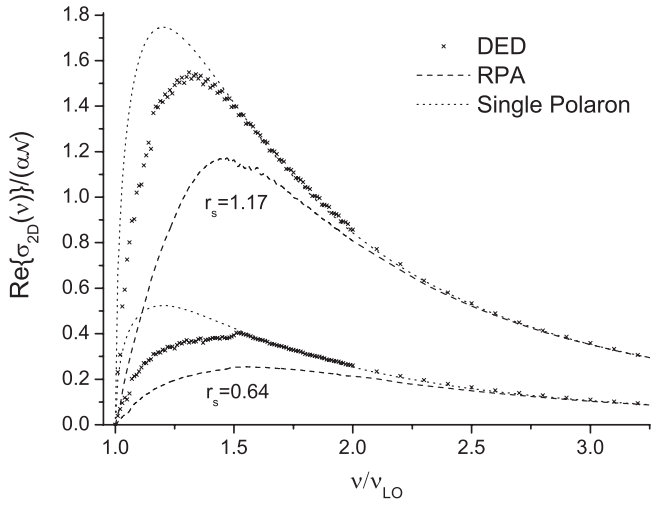

Fig. 4. The total optical absorption of a 2D many-polaron system in GaAs is shown as a function of the frequency ν in units of the LO phonon frequency $\nu_{\rm LO}$, for $r_s = 0.64$ (corresponding to $n = 10^{12}$ cm^{-2}) and $r_s = 1.17$ ($n = 3 \times 10^{11}$ cm^{-2}). Results are shown for the DED formalism (crosses), the RPA formalism (dashed curves) and for the single-polaron case (dotted curves). The noise present in the results is due to the numerical treatment. The delta-function in the optical absorption at $\nu = 0$ is not shown in this figure.

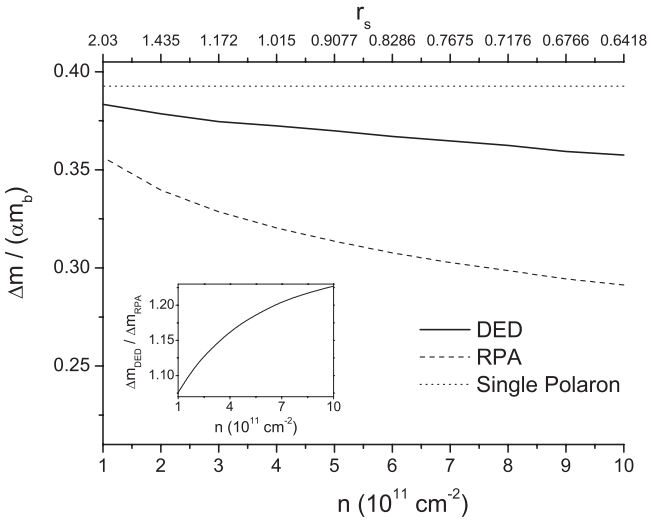

Fig. 5. The difference between the polaronic effective mass and the band mass $\Delta m = m^* - m_b$ is shown as function of the surface density n of the 2D polaron system in GaAs. The r_s values corresponding to the densities n are reported on the top axis. The DED result is plotted as a full curve, the RPA result as a dashed curve, and the one-polaron result as a dotted line. The inset shows the ratio between the effective mass enhancement in DED and RPA as a function of density.

total spectral weight is a constant:

$$\int_0^\infty \mathrm{Re}[\sigma(\omega)]d\omega = \frac{\pi N e^2}{2m_b}. \tag{14}$$

It is important to keep in mind that the optical absorption of the polaron system shows a delta-function in the origin ($\omega = 0$), not shown in Figure 4. The total spectral weight is distributed between this delta-function peak and the optical absorption spectrum beyond the single-phonon gap [25]. The spectral weight of the delta-function is related to the polaron effective mass m^* in such a way that [25]

$$\int_{\omega>\omega_{\rm LO}}^\infty \mathrm{Re}[\sigma(\omega)]d\omega = \frac{\pi N e^2}{2m_b}\left(1 - \frac{m_b}{m^*}\right). \tag{15}$$

Thus, a change in the spectral weight allotted to the $\omega > \omega_{\rm LO}$ region of the optical conductivity indicates a change in the effective mass of the polarons. The electron-phonon coupling increases the effective mass of a single polaron by $\Delta m = m^* - m_b$. The well-known single-polaron result for this effective mass increase in 2D is $\Delta m/m_b = \alpha\pi/8$. In Figure 5, we show the effective mass increase $\Delta m/(\alpha m_b) = (m^*/m_b - 1)/\alpha$ as a function of the surface density of polarons in GaAs. Both the RPA result (dashed curve, cf. [7–9,26]) and the DED result (full curve) approach the one-polaron result in the limit of small density. As the surface density of polarons increases, Δm decreases, more rapidly in RPA than in DED.

The fractional change $\Delta m_{\rm DED}/\Delta m_{\rm RPA}$ is shown in the inset of Figure 5, and indicates that there is roughly a 15% difference between the effective mass increase predicted by DED and that predicted by RPA. This is consistent with the increase in spectral weight of the optical absorption at $\omega > \omega_{\rm LO}$ in DED as compared to RPA: if less spectral weight is present in the region $\omega > \omega_{\rm LO}$, the delta-function in the origin must carry more spectral weight, indicating an increase in effective mass.

4 Ground-state energy of the interacting 2D polaron system

A general expression for the ground state energy per particle of an interacting polaron gas at weak coupling was derived in reference [6]:

$$E = E_{\rm el} - \sum_{\mathbf{q}} \frac{|V_{\mathbf{q}}|^2 S_{\rm 2D}(\mathbf{q})}{\hbar\omega_{\rm LO} + \dfrac{(\hbar q)^2}{2m_b S_{\rm 2D}(\mathbf{q})}}. \tag{16}$$

In this expression $E_{\rm el}$ is the energy contribution per particle of the system of charge carriers without electron-phonon coupling, and the second term is the polaron contribution. The 2D Fröhlich interaction amplitude appearing in this expression is

$$|V_{\mathbf{q}}|^2 = \frac{(\hbar\omega_{\rm LO})^2}{q}\frac{2\pi\alpha}{A}\sqrt{\frac{\hbar}{2m_b\omega_{\rm LO}}}, \tag{17}$$

with A the surface of the 2D system. Whereas the optical conductivity depends on the dynamic structure factor, the

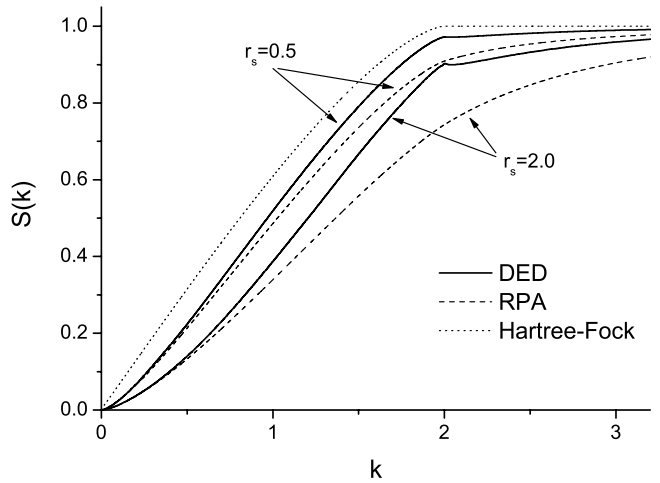

Fig. 6. The static structure factor of a 2D electron gas is shown as a function of the wave number k (in units of k_F), in the Hartree-Fock approximation (dotted curve), in RPA (dashed curves, at $r_s = 0.5$ and 2.0), and in DED (full curves, at $r_s = 0.5$ and 2.0).

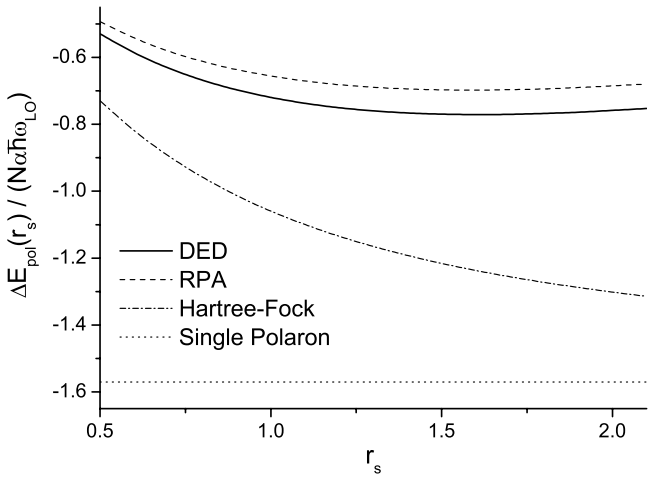

Fig. 7. The polaronic ground state energy in a 2D polaron system in GaAs is plotted as a function of r_s in the Hartree-Fock approximation (dash-dotted curve), in RPA (dashed curve) and in DED (full curve). The dotted line indicates the one-polaron result.

ground state energy depends on the static structure factor

$$S_{2D}(q) = \int_0^\infty \frac{d\omega}{\pi} S_{2D}(q,\omega) = -\frac{\hbar}{n\pi v_q} \int_0^\infty \mathrm{Im}\left(\frac{1}{\varepsilon\,(q,\omega)}\right) d\omega. \qquad (18)$$

Expressed in dimensionless variables for the wave number and the frequency, this is

$$S_{2D}(k) = -\frac{\sqrt{2}k}{\pi r_s} \int_0^\infty \mathrm{Im}\left(\frac{1}{\varepsilon\,(k,\nu)}\right) d\nu. \qquad (19)$$

A comparison between the static structure factor in RPA and DED is shown in Figure 6. Around $k = 2$, the DED static structure factor shows a transition to the long wave length behavior [18,19].

The shift in ground state energy per particle due to the electron-phonon coupling $\Delta E_{\mathrm{pol}} = E(\alpha) - E(\alpha = 0)$ is given by [6]:

$$\Delta E_{\mathrm{pol}} = -\alpha\hbar\omega_{\mathrm{LO}} \int_0^\infty dk\ \gamma \frac{[S_{2D}(k)]^2}{S_{2D}(k) + \gamma^2 k^2}. \qquad (20)$$

with $\gamma = k_F/k_{\mathrm{LO}}$ and $k_{\mathrm{LO}} = \sqrt{2m_b\omega_{\mathrm{LO}}/\hbar}$. The result for the polaronic shift in the ground state energy per particle, as a function of the Wigner-Seitz radius r_s, is shown in Figure 7 for different approaches. The material parameters for GaAs were used for this figure. If no many-body effects are taken into account, the 2D polaronic energy per particle is $-(\pi/2)\alpha\hbar\omega_{\mathrm{LO}}$ in the weak coupling regime. If many-body effects are taken into account on the level of the Hartree-Fock approximation, we get a monotonous decreasing energy as r_s increases, while the RPA approximation leads to a minimum in the polaronic energy at $r_s = 1.59$, with $E/N = -0.70\ \alpha\hbar\omega_{\mathrm{LO}}$. We find that including dynamical exchange effects lowers $|\Delta E_{\mathrm{pol}}|$ with respect to RPA, and shifts the energy minimum to slightly lower density: $r_s = 1.61$, where $E/N = -0.77\ \alpha\hbar\omega_{\mathrm{LO}}$. So, using an improved dielectric function as compared to RPA leads to a change of ca. 10% in the ground state energy.

5 Conclusions

Efforts to describe many-body effects in the polaron system have thus far relied strongly on the RPA approach [6–9,15,23], even though there have been indications that inclusion of a *static* local field correction modifies the ground state energy and the effective mass of the polarons [10]. In this paper, we use a dielectric function that includes a *frequency-dependent* local field correction derived in the time-dependent Hartree-Fock formalism [17–19]. We find that taking into account dynamical exchange effects reveals important corrections at weak coupling to the optical absorption of the polaron system, the effective mass of the polarons and the ground state energy of the polaron system. In GaAs, estimates of the effective mass based on RPA are roughly 15% off from the improved results, estimates of the ground state energy differ roughly 10%. Furthermore, we show that in the optical absorption, RPA considerably overestimates the reduction of spectral weight due to the many-body effects.

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24. Note that the single-polaron results can be obtained by using an effective loss function $-\mathrm{Im}[1/\varepsilon] = [\pi r_s/(\sqrt{2}k)]\delta(\nu - k^2/2)$. The delta-function fixes the free-particle dispersion, whereas the proportionality factor ensures that the sum rules are satisfied
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