Two-dimensional electron gas in the random-phase approximation with exchange and self-energy corrections

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We determine a dynamical field correction of the two-dimensional electron gas, taking into account exchange and self-energy contributions to the random-phase approximation (RPA). Physical properties like correlation energy, electron self-energy, effective mass, quasiparticle renormalization factor, and momentum distribution are computed. With respect to the RPA, we find a substantial reduction of the correlation energy, whereas the electron effective mass is much less affected.

I. INTRODUCTION

The two-dimensional electron gas has recently gained much interest mostly because of the advent of high-T_c superconductivity. In this article we consider the two-dimensional electron gas in its continuum version (jellium model).[1–3] The aim of the present work is in fact rather modest, trying to assess the validity of an approximation proposed long ago[4,5] to treat exchange and self-energy corrections beyond the standard random-phase approximation (RPA). Such simplifying approximations are quite important because even the simplest extension of the RPA, namely, the inclusion of exchange and self-energy corrections, leads to a rather inextricable integral equation that will be detailed later. As we will demonstrate, the proposed approximation turns out to work very well indeed, reducing the numerical effort drastically to a (four-dimensional) quadrature. We can thus set up the framework for a more exact and elaborate approach beyond the RPA that we envisage for the future.[6]

An additional simplification stems from the fact that we will only treat the charge response function, postponing the spin response to future work. We write the density-density response function as the formally exact expression

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1-[1-G(q,\omega)]v_q\chi_0(q,\omega)}, \tag{1}$$

where $v_q=2\pi e^2/q$ is the Coulomb potential and χ_0 is the Lindhard function in two dimensions. The unknown is now the so-called field correction $G(q,\omega)$. Neglecting it altogether leads to the well-known standard RPA (ring summation). This field correction becomes increasingly important for small densities, or large ($\gtrsim 1$) values of the parameter $r_s=\sqrt{2}me^2/k_F$ with k_F the electron Fermi momentum. Of course, just like χ, G possesses a well-defined perturbation series in powers of the coupling constant e^2. Our aim here is to evaluate G to lowest order in the coupling constant, and in fact it has already a contribution to zeroth order coming from the ''exchange conjugate'' diagrams to the RPA, which in its simplest form was estimated by Hubbard[7]:

$$G_H(q)=\frac{1}{2}\frac{q}{\sqrt{q^2+k_F^2}}. \tag{2}$$

It can be seen that for large momenta the interaction is weakened by a factor 1/2, accounting for the influence of the Pauli principle. Static expressions based on this one have been investigated by a number of authors.[8–10] Recently, also the complete inclusion of exchange and self-energy parts into the RPA by solving the corresponding integral equation has been presented in the literature.[11–13]

The two-dimensional (2D) electron gas can actually be considered as a benchmark system since there exist quantum Monte Carlo (QMC) results for various observables,[14–16] against which approximate solutions can be tested. We will show that our approximation scheme considerably improves the prediction of physical properties like correlation energy and single-particle properties of the system with respect to the conventional RPA.

II. FORMALISM

An exact formulation of exchange contributions to the RPA can be found in Refs. 4 and 11, for example. One writes (we use $\hbar=1$ in the following)

$$\chi(\boldsymbol{q},\omega)=2\int\frac{d^2p}{(2\pi)^2}f(\boldsymbol{p},\boldsymbol{q},\omega)D_0(\boldsymbol{p},\boldsymbol{q},\omega) \tag{3}$$

with the free particle-hole propagator

$$D_0(\boldsymbol{p},\boldsymbol{q},\omega)=\frac{n(\boldsymbol{p}_-)-n(\boldsymbol{p}_+)}{e(\boldsymbol{p}_-)-e(\boldsymbol{p}_+)+\omega+\mathrm{sgn}(\omega)i\epsilon}, \tag{4}$$

where $n(\boldsymbol{k})=\theta(k_F-k)$, $e(\boldsymbol{k})=k^2/2m$, and we have introduced the notation $\boldsymbol{p}_\pm=\boldsymbol{p}\pm\boldsymbol{q}/2$. The vertex function f is the solution of the integral equation[4,17]

$$f(\boldsymbol{p},\boldsymbol{q},\omega)=1-\frac{\Sigma_F(\boldsymbol{p}_-)-\Sigma_F(\boldsymbol{p}_+)}{e(\boldsymbol{p}_-)-e(\boldsymbol{p}_+)+\omega}f(\boldsymbol{p},\boldsymbol{q},\omega)+2\int\frac{d^2k}{(2\pi)^2}V(\boldsymbol{p},\boldsymbol{k},\boldsymbol{q})D_0(\boldsymbol{k},\boldsymbol{q},\omega)f(\boldsymbol{k},\boldsymbol{q},\omega) \tag{5}$$

with the interaction kernel

$$V(\boldsymbol{p},\boldsymbol{k},\boldsymbol{q})=2\pi e^2\left(\frac{1}{q}-\frac{1}{2}\frac{1}{|\boldsymbol{p}-\boldsymbol{k}|}\right) \tag{6}$$

and the Fock electron self-energy

$$\Sigma_F(\boldsymbol{p})=-\int\frac{d^2k}{(2\pi)^2}n(\boldsymbol{k})\frac{2\pi e^2}{|\boldsymbol{p}-\boldsymbol{k}|}. \tag{7}$$

Graphical representations of Eqs. (3) and (5) are given in Refs. 11 and 12. Physically, the second term on the right-hand side (rhs) of Eq. (5) originates from the Fock correction to the electron self-energy in the denominator of the particle-hole propagator [see Eq. (4)], whereas the third one includes the vertex correction due to the exchange diagram of the particle-hole interaction. There is a strong cancellation between the two contributions that can be made explicit by combining the two terms in the form

$$f(\boldsymbol{p})=1-4\pi me^2\widetilde{\sum_k}\left[\frac{1}{q}\frac{f(\boldsymbol{k})}{\boldsymbol{k}\cdot\boldsymbol{q}-m\omega}-\frac{1}{2}\frac{1}{|\boldsymbol{p}-\boldsymbol{k}|}\times\left(\frac{f(\boldsymbol{k})}{\boldsymbol{k}\cdot\boldsymbol{q}-m\omega}-\frac{f(\boldsymbol{p})}{\boldsymbol{p}\cdot\boldsymbol{q}-m\omega}\right)\right], \tag{8}$$

where we have defined

$$\widetilde{\sum_k}\equiv\int\frac{d^2k}{(2\pi)^2}[n(\boldsymbol{k}_-)-n(\boldsymbol{k}_+)] \tag{9}$$

and we have not explicitly indicated the dependence of f on $(\boldsymbol{q},\omega)$. It can be seen that the singular structure (for $\boldsymbol{k}\to\boldsymbol{p}$) of the kernel in Eqs. (5) and (6) is artificial and removed in Eq. (8). The latter variant is therefore more suitable for a numerical treatment.

Still, the full numerical solution of Eq. (8) is a difficult task, which has been attempted in Refs. 11–13. Here, we will perform it only for the static case ($\omega=0$), in order to compare with an approximate solution, mentioned in the introduction, that turns out to be very accurate. Expanding Eq. (1) and iterating Eqs. (3) and (8) once, one can identify an approximate expression for the field correction that corresponds to its exact result to zeroth order in the interaction[4,5,18]:

$$G(q,\omega)=\frac{\frac{q}{2}\widetilde{\sum_p}\left[\frac{1}{[\boldsymbol{p}\cdot\boldsymbol{q}-m\omega]^2}\widetilde{\sum_k}\frac{\boldsymbol{q}\cdot\boldsymbol{e}_{\boldsymbol{p}-\boldsymbol{k}}}{\boldsymbol{k}\cdot\boldsymbol{q}-m\omega}\right]}{\left[\widetilde{\sum_p}\frac{1}{\boldsymbol{p}\cdot\boldsymbol{q}-m\omega}\right]^2} \tag{10}$$

with $\boldsymbol{e}_{\boldsymbol{p}-\boldsymbol{k}}=(\boldsymbol{p}-\boldsymbol{k})/|\boldsymbol{p}-\boldsymbol{k}|$. It is convenient to introduce the dimensionless variables $x=q/2k_F$ and $y=m\omega/2k_F^2$. Then, G is explicitly given by

$$G(x,y)=\frac{1}{\widetilde{\int_p}2}\widetilde{\int_p}\widetilde{\int_k}\frac{x^2}{xu_p\cos\phi_p-y}\times\frac{u_p\cos\phi_p-u_k\cos\phi_k}{\sqrt{u_p^2+u_k^2-2u_pu_k\cos(\phi_p-\phi_k)}} \tag{11}$$

with

$$\widetilde{\int_p}=\left(\int_0^{\phi_{\max}}-\int_{\pi-\phi_{\max}}^{\pi}\right)d\phi_p\int_{u_{\min}(\phi_p)}^{u_{\max}(\phi_p)}du_p\frac{u_p}{xu_p\cos\phi_p-y}, \tag{12}$$

$$\phi_{\max}=\arcsin[\min(1/x,1)], \tag{13}$$

$$u_{\max,\min}(\phi)=|x\cos\phi\pm\sqrt{1-(x\sin\phi)^2}|. \tag{14}$$

Written in this form, one notes in particular that the approximate field correction [as the Hubbard approximation Eq. (2)] depends only on the scaled variables x and y, and not on the parameter r_s, i.e., on density or in particular on the strength of the interaction, e.

This approximation, termed (perturbative) RPAE in the following, was first derived in Ref. 4 within a variational approach, and analytical solutions for limiting cases were considered. The term RPAE (RPA with exchange, see, e.g., Ref. 11) is retained for historical reasons: however, by mentioning here and elsewhere the exchange contribution we mean that also the self-energy contributions are included. In Ref. 18 a closely related approximation was obtained within a perturbative expansion of the proper polarization up to first order in the coupling constant. In this work we will evaluate Eq. (11) numerically by integration in order to compute various physical quantities. Since the integrands appearing in that equation are singular, a numerical evaluation is still delicate.[18] However, for many applications it is sufficient to know the field correction for purely imaginary values of the energy variable, $\omega=iu$. Then the numerical treatment of Eqs. (8) and (10) is more reliable and, in addition, G is purely real.

III. RESULTS

A. Field correction

We begin the discussion of our results with the static case $\omega=0$. Figure 1 displays the field correction G (independent of r_s) and the response functions χ for $r_s=1$ and $r_s=5$. We compare with numerical results of the full integral equation for $r_s=1$, which were obtained by discretization and diagonalization of Eq. (8) and subsequent numerical integration of Eq. (3). It can be seen that the approximation Eq. (10) is very good, apart from a small region around $x=1$. Here one observes in both cases a peak which is even more pronounced for the full solution. It was also noted in Ref. 18, but not in Refs. 11–13, apparently due to a limited numerical accuracy.

Since in the region around $x=1$ the field correction reaches values larger than 1, it is clear that for sufficiently large r_s the response function Eq. (1) develops two singularities. Using $v\chi_0(x=1,y=0)=-r_s/\sqrt{2}$ and our numerical

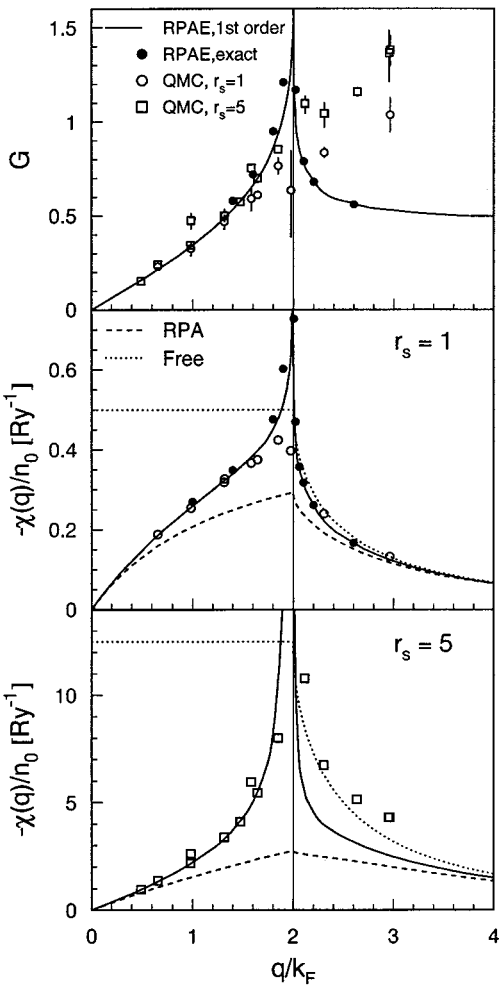

FIG. 1. The static field correction $G(q,\omega=0)$ and the corresponding response functions for $r_s=1$ and $r_s=5$. (Normalization $n_0=k_F^2/2\pi$.) The dashed curves denote standard RPA results, the full curves the results of the approximation Eq. (10), and the solid markers the exact solutions of Eq. (5) for $r_s=1$. The values for free particles, i.e., $\chi=\chi_0$, are displayed as dotted lines. We compare with QMC results of Ref. 14 (open markers).

result for the peak height, $G(1,0)\approx 1.8$ (which is in good agreement with the value 1.803 given in Ref. 18), this happens for $r_s \gtrsim 1.76$. In the equivalent investigation of Ref. 17 for the three-dimensional case this fact was interpreted as an instability of the ground state toward formation of charge-density waves. It should be noted here that, taking as criterion the positiveness of the pair correlation function, the RPAE breaks down much earlier, namely, at $r_s\approx 0.7$, as shown in Ref. 18. For the exact solution of the RPAE the problem is even more severe, since the peak is more pronounced, which renders a precise numerical solution extremely difficult.[17] We have therefore only performed the comparison at $r_s=1$. Results for larger values of r_s were given in Ref. 11; however, as noted above, the numerical accuracy appears quite limited in that case and the peak is not resolved.

However, we think that this peak can be considered as an artifact of the standard RPA approximation scheme where one assumes sharp momentum distribution functions, and we have verified that its influence on bulk properties is very small. This conclusion stems from the results of a recent work,[6] where ground-state correlations smoothed out the occupation numbers and consequently cusps and singularities due to the sharp edge of the Fermi sphere were washed out. In Ref. 17 the problem was tackled in a related way by introducing (in an *ad hoc* manner) Thomas-Fermi screening of the interaction. The peak is clearly a signal for the need of setting up an approximation scheme beyond the RPAE, which we intend to prepare in this article.

In any case, apart from the region $x\approx 1$ the resulting observables are well behaved, and we give in Fig. 1 a comparison with quantum Monte Carlo results.[14] Apparently, for $q<2k_F$ the RPAE is in close agreement with the QMC results at $r_s=1$ and $r_s=5$, whereas for larger momenta there seems to be a substantial discrepancy, the QMC calculation predicting a nearly linear increase with momentum q. This is indeed the limiting behavior expected theoretically for $q\to\infty$.[19] In Ref. 12 a large part of this difference between RPAE and QMC results was attributed to particle-particle correlations by taking into account ladder diagrams of the electron-electron interaction. Unfortunately, at present the accuracy of the QMC results is not high enough[20] to decide on the behavior (enhancement) near $q=2k_F$.

For nonzero (imaginary) ω the variation of G is smoothed out and the peak at $q=2k_F$ disappears. This can be seen in Fig. 2, where G is shown as function of x and imaginary y. From the expression Eq. (10) one can derive the limiting values

$$G(x,y)\to\begin{cases} 1/2, & x\to\infty \\ 2x/\pi, & x\to 0, \quad y=0 \\ 5x/3\pi, & x\to 0, \quad y\to i\infty, \end{cases} \tag{15}$$

which remain valid for the exact solution of Eq. (8).[4] The simplest static Hubbard approximation according to Eq. (2), which is also displayed in the figure, does not reproduce either the correct slope for small x, or the enhancement around $x=1$.

Having the field correction at our disposal, several physical properties of the electron gas can be calculated.

B. Correlation energy

We begin with the correlation energy,[7,13,21–25]

$$E_c = R_\infty \frac{16}{\pi r_s^2}\int_0^\infty dx x \int_0^\infty dy \times\left[\frac{\ln[1-(1-G)v\chi_0]}{1-G}+v\chi_0\right](x,iy), \tag{16}$$

where $R_\infty=13.606$ eV is the Rydberg energy and the Lindhard function χ_0 for imaginary energy is given by[26]

$$v\chi_0(x,iy)=-\frac{r_s}{\sqrt{2}x}\left(1-\frac{1}{x}\mathrm{Re}\sqrt{z^2-1}\right), \quad z=i\frac{y}{x}-x. \tag{17}$$

Note that in order to arrive at the expression Eq. (16), an integration over the strength of the interaction was performed (charging procedure).[1,2,7,21,23] This is only possible if the field correction does not depend on e, as in our approxi-

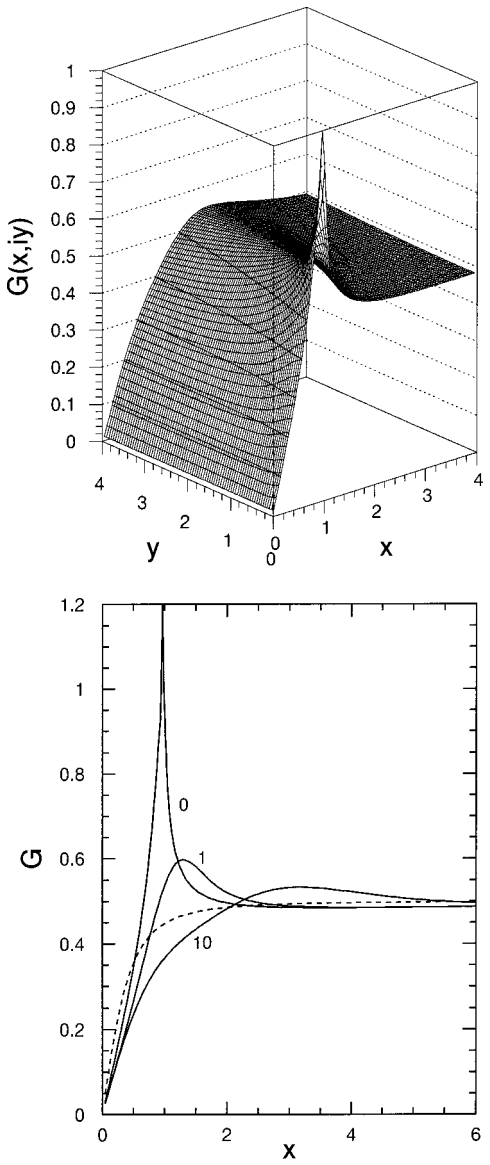

FIG. 2. The field correction G as a function of momentum, $x=q/2k_F$, and imaginary energy, $y=m\omega/2k_F^2$ (top panel). The lower panel shows the results for selected values of $y=0,1,10$. For comparison the result of the Hubbard approximation, Eq. (2), is shown as a dashed curve.

mation. It is important to point out that Eq. (16) cannot be used with the solution of the full equation (5), since then G contains all powers of the interaction and consequently depends on the coupling constant.

Our results (RPAE) are given in Table I and compared with those of the standard RPA, the simplest Hubbard approximation, Eq. (2), and QMC results of Ref. 15. We find that the exchange contributions reduce significantly (in magnitude) the correlation energy, bringing it close to the QMC results. This reduction is due to the effective weakening of the bare interaction by the exchange effect, and we find a stronger reduction than with the Hubbard approximation, consistent with the fact that the exact calculation yields an overall larger field correction (see Fig. 2). In Ref. 13 an even stronger reduction of the correlation energy was reported with the full solution of the integral equation (5). However, in that reference the expression Eq. (16) was used in spite of the remarks made above.

C. Effective mass

A quantity of central interest is the electron self-energy. Here, one obtains after a Wick rotation to the imaginary ω axis the well-known expression[22,26–28]

$$\Sigma(k,e)=-\sum_q\left[\frac{v_q}{2}+V_s(q,e_{k+q}-e)[\theta(e_F-e_{k+q})-\theta(e-e_{k+q})]+\int_{-\infty}^{+\infty}\frac{du}{2\pi}\frac{V_s(q,iu)}{iu+e-e_{k+q}}\right], \tag{18}$$

where the screened interaction V_s is given by the prescription of Rice,[22,29] consistent with the expression for the correlation energy, Eq. (16):

$$V_s(q,\omega)=\frac{v_q}{\epsilon_s(q,\omega)}=\frac{v_q}{1-[1-G(q,\omega)]v_q\chi_0(q,\omega)}. \tag{19}$$

The second term on the rhs in Eq. (18) requires the knowledge of ϵ_s for real values of the energy variable ω. However, it vanishes for $e=e_F$. In particular, one obtains for the on-shell self-energy on the Fermi line,[26]

TABLE I. Properties of the two-dimensional electron gas as a function of the density parameter r_s. RPA denotes standard RPA results, RPAH the Hubbard approximation according to Eq. (2), RPAE the approximation Eq. (10), and QMC the results of Ref. 15.

	$-E_c$ (eV)				$-\Sigma_c$ (eV)		$-\partial\Sigma/\partial e$		$m/k_F\partial\Sigma/\partial k$		$(m^*/m)_{\text{pert.}}$		$(m^*/m)_{\text{s.c.}}$		Z	
r_s	RPA	RPAH	RPAE	QMC	RPA	RPAE	RPA	RPAE	RPA	RPAE	RPA	RPAE	RPA	RPAE	RPA	RPAE
0.5	6.27	4.19	3.83	3.64	6.84	3.61	0.27	0.25	0.30	0.29	0.977	0.964	0.981	0.971	0.786	0.799
1.0	5.39	3.65	3.32	2.98	6.07	3.28	0.51	0.46	0.48	0.46	1.030	1.006	1.020	1.003	0.662	0.683
2.0	4.41	3.05	2.76	2.26	5.13	2.87	0.93	0.83	0.79	0.71	1.163	1.126	1.078	1.065	0.519	0.548
3.0	3.83	2.68	2.43	1.84	4.54	2.61	1.29	1.14	1.05	0.92	1.315	1.276	1.117	1.112	0.437	0.468
4.0	3.43	2.42	2.20	1.55	4.11	2.42	1.61	1.42	1.28	1.11	1.485	1.452	1.143	1.148	0.383	0.414
5.0	3.13	2.23	2.03	1.35	3.79	2.27	1.91	1.67	1.50	1.28	1.682	1.661	1.162	1.175	0.344	0.374
8.0	2.54	1.84	1.68	0.98	3.13	1.96	2.70	2.34	2.09	1.73	2.537	2.620	1.196	1.227	0.270	0.299
10.0	2.29	1.67	1.53	0.83	2.84	1.81	3.17	2.74	2.45	2.00	3.573	3.855	1.209	1.247	0.240	0.268

$$\Sigma(k_F,e_F)=\Sigma_F(k_F)\left[1+\int_0^\infty dx\int_0^\infty\frac{dy}{x}\left(\frac{1}{\epsilon_s(x,iy)}-1\right)\times\mathrm{Re}\left(\frac{1}{\sqrt{z^2-1}}\right)\right] \tag{20}$$

$$\equiv\Sigma_F+\Sigma_c, \tag{21}$$

where z was given in Eq. (17), $\Sigma_F\equiv\Sigma_F(k_F)=-R_\infty 4\sqrt{2}/\pi r_s$ is the Fock part of the electron self-energy [see Eq. (7)], and we have defined the correlation part on the Fermi line, Σ_c.

In a similar manner one can calculate the quantities

$$\frac{\partial\Sigma}{\partial e}(k_F,e_F)=+\frac{r_s}{\pi\sqrt{2}}\int_0^\infty\frac{dx}{x}\int_0^\infty\frac{dy}{x}\times\left(\frac{1}{\epsilon_s(x,iy)}-\frac{1}{\epsilon_s(x,0)}\right)\mathrm{Re}\left(\frac{z}{(z^2-1)^{3/2}}\right), \tag{22a}$$

$$\frac{m}{k_F}\frac{\partial\Sigma}{\partial k}(k_F,e_F)=-\frac{r_s}{\pi\sqrt{2}}\int_0^\infty\frac{dx}{x}\int_0^\infty\frac{dy}{x}\times\frac{1}{\epsilon_s(x,iy)}\mathrm{Re}\left(\frac{z+2x}{(z^2-1)^{3/2}}\right), \tag{22b}$$

which serve to determine the effective mass m^* of the electrons. However, on this topic there exists in the literature a long-standing discussion[3,22,29,30] whether m^* should be determined from the Dyson equation,

$$E_k=e_k+\Sigma(k,e), \tag{23}$$

in a ''perturbative'' ($e=e_k$) or ''self-consistent'' ($e=E_k$) fashion. Since this question can ultimately be resolved only by calculating explicitly the relevant contributions to Σ beyond the RPA, we present in the following results for both prescriptions, namely,

$$\left(\frac{m^*}{m}\right)_{\text{pert.}}=\frac{1}{1+\partial\Sigma/\partial e+(m/k_F)(\partial\Sigma/\partial k)}, \tag{24a}$$

$$\left(\frac{m^*}{m}\right)_{\text{s.c.}}=\frac{1}{Z}\frac{1}{1+(m/k_F)(\partial\Sigma/\partial k)},\quad Z=\frac{1}{1-\partial\Sigma/\partial e}, \tag{24b}$$

in the perturbative and in the self-consistent scheme, respectively.

Our results for the various quantities are shown in Table I and Fig. 3. One notes that the e and k derivatives of the self-energy are both large and strongly compensate each other for the physical effective mass. In the RPAE both contributions are reduced in size, but their sum is much less affected and the effective mass remains therefore nearly the same as in the standard RPA. Our results are in qualitative agreement with those of Refs. 10,29–31, whereas QMC calulations[16] predict much smaller effective masses close to unity. The difference between the perturbative and self-consistent determination of the effective mass is slightly reduced in the RPAE. However, it is still quite large and increases with decreasing density. This variance is due to the magnitude of the quasiparticle renormalization factor Z which decreases rapidly with increasing r_s, attaining values below 0.4 at $r_s=5$. This points to the importance of including into the formalism in a consistent manner the modification of the momentum distribution as suggested in Ref. 6.

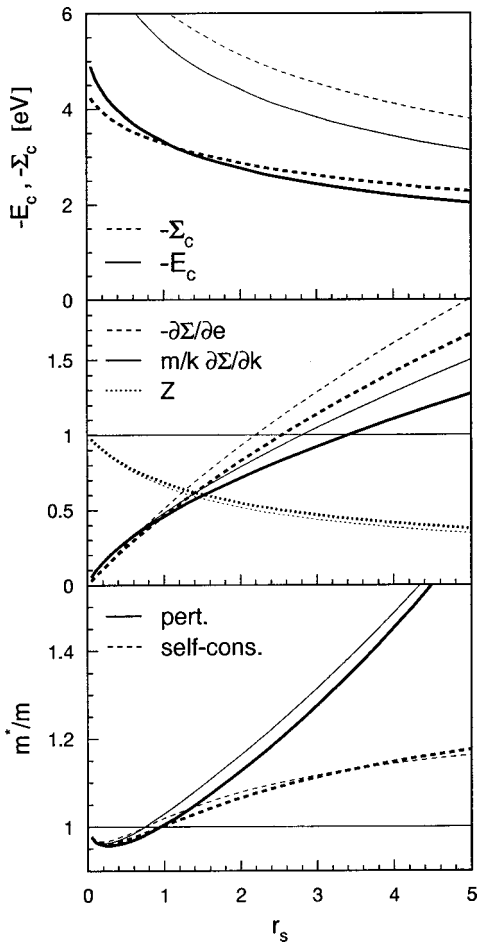

FIG. 3. Various quantities as a function of the density parameter r_s. The standard RPA results are plotted using thin lines; the RPAE results with thick lines. Top panel: Correlation energy E_c and correlation part of the electron self-energy at the Fermi line Σ_c. Central panel: k and e derivatives of the electron self-energy, and quasiparticle renormalization factor Z. Bottom panel: The electron effective mass m^* in two different approximations, according to Eq. (24).

D. Momentum distribution

As a first step toward such an extension we compute the momentum distribution within an approach that was first applied to the three-dimensional case in Ref. 32. It has the advantage that it requires, like the quantities considered so far, the polarization function and field correction only for purely imaginary energies.

The method consists in considering a fictive Hamiltonian with a modified kinetic term:

$$\hat{H}=2\sum_p\left[\frac{p^2}{2m}+\lambda\,\delta(|\boldsymbol{p}|-k)\right]\hat{n}_p+\hat{H}_{\text{int}}. \tag{25}$$

The shift of the energy per electron caused by the (infinitesimal) additional term is therefore $E_\lambda(k)=\lambda(2k/k_F^2)n(k)$, where $n(k)$ is the momentum distribution of the interacting system. On the other hand in the RPAE this shift can be computed explicitly from Eq. (16) by inserting the modified single-particle energy in the denominator of Eq. (4) and subsequently expanding Eq. (3) for χ_0 (i.e., setting $f=1$) and Eq. (16) for E_c to first order in λ. In this way one obtains for the momentum distribution

$$n(k)-1=\frac{r_s}{\sqrt{2}\pi^2\kappa^2}\int_{(1-\kappa)/2}^{\infty}\frac{dx}{x}\int_0^{\infty}\frac{dy}{x}\,\frac{1}{\epsilon_s(x,iy)} \times \mathrm{Re}[F(\alpha,z/\kappa)] \quad (k<k_F), \tag{26a}$$

$$n(k)=\frac{r_s}{\sqrt{2}\pi^2\kappa^2}\int_{(\kappa-1)/2}^{(\kappa+1)/2}\frac{dx}{x}\int_0^{\infty}\frac{dy}{x}\,\frac{1}{\epsilon_s(x,iy)} \times \mathrm{Re}[F(\alpha,z/\kappa)-F(\pi,z/\kappa)] \quad (k>k_F) \tag{26b}$$

with $\kappa=k/k_F$,

$$\alpha=\begin{cases}\arccos\left(\dfrac{1-4x^2-\kappa^2}{4x\kappa}\right), & x<(1+\kappa)/2\\ \pi, & x>(1+\kappa)/2,\end{cases} \tag{27}$$

and

$$F(\alpha,z)=\int_0^{\alpha}d\phi\,\frac{1}{(z-\cos\phi)^2} =\frac{2z}{(z^2-1)^{3/2}}\arctan\left(\sqrt{\frac{z+1}{z-1}}\tan\frac{\alpha}{2}\right) +\frac{1}{z^2-1}\,\frac{\sin\alpha}{z-\cos\alpha}. \tag{28}$$

In the limit $k\to k_F$ one obtains in this approach $n(k_F-0)-n(k_F+0)=-\partial\Sigma/\partial e(k_F,e_F)$, as given in Eq. (22a). Consequently the method is valid in the limit of weak perturbation, namely, if $Z=(1-\partial\Sigma/\partial e)^{-1}\approx 1+\partial\Sigma/\partial e$.

Figure 4 shows the results with and without exchange correction at $r_s=1$ and 2. Again the weakening of the interaction when exchange is included leads to a smaller deviation from the undisturbed Fermi distribution than in the standard RPA case.

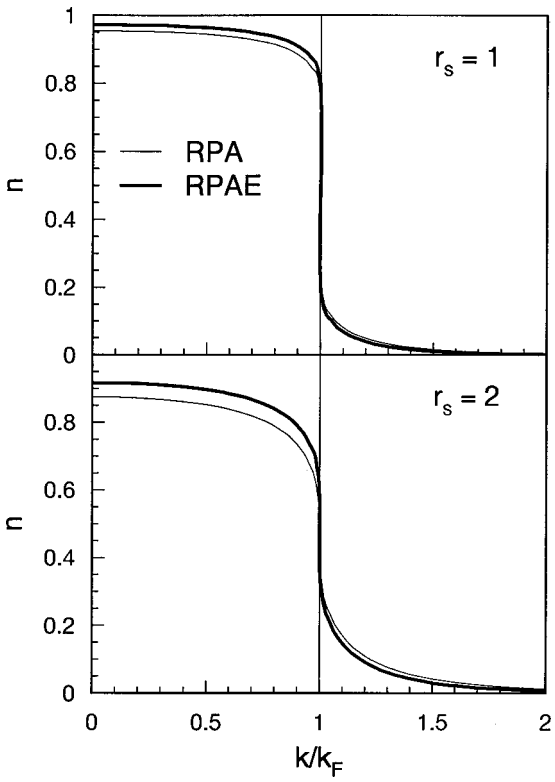

FIG. 4. Momentum distributions in RPA (thin lines) and RPAE (thick lines) for $r_s=1,2$.

IV. CONCLUSIONS

In this work we have considered self-energy and exchange corrections to the standard RPA (ring summation) for the two-dimensional electron gas in the jellium model. A strong mutual cancellation of the two effects was pointed out explicitly. We considered the charge response function and treated the exchange terms approximately by a systematic renormalization of the direct interaction term. We found that, for not too small density ($r_s\lesssim 1$) at least, on the one hand our approach for the response function approximates the exact treatment of exchange very well, and on the other hand it brings the solution much closer to the exact values known from recent QMC results. Also, for the correlation energies one notes that our approach works very well at higher densities ($r_s\lesssim 1$), greatly improving the standard RPA.

Clearly at lower densities still some correlations are missed; also the RPA-like formalism becomes problematic due to the appearance of singularities in the response function. All this hints of the necessity of going beyond the RPA + exchange approach. In this respect it has recently been shown that the so-called self-consistent RPA can give interesting results. (See Ref. 6 and works cited there.) A simpler version, the so-called renormalized RPA, where only the occupation numbers are calculated self-consistently using the RPA screened exchange potential in the single-particle Dyson equation, seems particularly promising in the present context and will be studied in future work. As a first step, we presented the occupation numbers of the 2D electron gas in the RPA(E). For the future we envisage establishing a self-consistent scheme by utilizing the corrected momentum distribution for the computation of a more realistic Lindhardt function and the quantities that are based on it.

Concerning the single-particle properties, we found that the electron effective mass is quite insensitive to the inclusion of exchange. A fundamental problem persists in the correct manner of evaluating the effective mass, which, together with the smallness of the quasiparticle renormalization factor, points again to the necessity of going beyond the RPA + exchange approach.

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