The electron effective mass in the strongly correlated 2D-uniform electron fluid from finite-temperature calculations.

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I. INTRODUCTION.

At very low temperatures, essentially at $T = 0$, the electrons in a 2D uniform electron fluid (UEF) occupy momentum states up to the Fermi energy $E_F$. If the electrons were non-interacting they have only kinetic energy, the potential energy being a constant. The energy bands of the electrons are of the form $k^2/2m$, where the mass $m$ of the non-interacting electrons is unity, even in semiconductor nanostructures or metals where the material parameters can be subsumed by a suitable re-definition of the effective atomic units [5]. Such 2D electron layers have been experimentally realized in semiconductor interfaces, enabling the experimental probing of such systems which are of great fundamental and technical importance.

If the number of electrons in a unit area (measured in atomic units) is $n$, the radius of the disk in real space per electron, viz. $r_s$, is $1/\sqrt{(\pi n)}$. The ratio of the Coulomb interaction to the kinetic energy is a measure of the ‘strength’ of the interactions in the system. In the limit $T \to 0$ it is found to be equal to $r_s$. Thus $r_s$ plays the role of the ‘expansion parameter’ or coupling constant in the perturbation theories of the electron fluid. Perturbation theories work reliably when the coupling $r_s$ is less than unity. The range of validity can sometimes be increased by the use of a ‘screened interactions’, at least for some properties.

One of the tenets of Fermi liquid theory, originally developed to treat the behaviour of electrons in metals (where usually $2 < r_s < 5$), is that the low-energy excitations in these interacting systems, known as quasi-particles, are very similar to non-interacting electrons. However, the mass $m$ is replaced by an effective mass $m^*$ which allows for the modification of the energy bands due to many-body interactions. Other parameters which describe the electrons, e.g., the Landé $g$ factor, are also modified and these are the ‘Fermi-liquid parameters’ of Landau theory. Unfortunately, standard many-body theory which uses perturbation methods cannot make a reliable evaluation of $m^*$ for systems where $r_s$ is greater than unity. Physically motivated approximations are needed to truncated the perturbation chain, and these invariably result in the failure to satisfy the sum rules, self-consistency conditions etc. If the results were insensitive to the various possible choices for screening, vertex corrections, selection of graphs, etc., then this would not matter. Unfortunately, the evaluation of $m^*$, usually carried out from a physically motivated approximation to the self energy, turns out to be very sensitive to the model used. Thus, for example, perturbation theories may predict the $m^*$ of electrons at $r_s=5$ to be a fraction of the bare mass, or several times the bare mass, depending on the model used. These methods even fail to predict positive-definite pair-distribution functions (PDFs), i.e., $g(r)$ for useful values of $r_s$.

However, significantly more reliable results are available from quantum Monte Carlo simulations (QMC), especially for PDFs and correlation energies. Unfortunately, the $m^*$ evaluations involve the probing of excited states, and only a few QMC calculations are available for the effective mass of the 2D UEF. Experimentally too, the measurements have been very challenging. Neverth-
less, currently available results, both experimental and simulational, show that the \( m^* \) of the 2D-paramagnetic electron liquid is enhanced above unity as \( r_s \) increases, while the \( m^* \) of the fully spin-polarized system remains below unity even as \( r_s \) is increased.

An alternative approach to the study of the effective mass is to look at quasiparticle excitations in a fluid at a temperature \( T \) close to \( T = 0 \). The thermal excitations occur in a strip of energy of width \( T \) near \( E_F \). The excitations in the system are associated with an increase in the Helmholtz free energy \( F_0 \) (non-interacting case), or \( F \) (interacting case), of the system. The quasiparticle mass enters directly into the specific heat of the system. Hence the ratio of the specific heats of the interacting and non-interacting systems provides a direct and unambiguous measure of the effective mass \( m^* \) of the excitations. Under certain conditions, these can be identified with the Landau quasiparticles of the Fermi liquid in the limit \( T \rightarrow 0 \) as discussed by Luttinger and others [2]. Thus a calculation of the interacting free energy \( F \) as a function of \( r_s \) at finite-\( T \) would provide an estimate of the effective mass \( m^* \), if the finite-\( T \) free-energy of the system could be calculated.

The calculation of the finite-\( T \) interacting free energy or the self-energy at the Hartree-Fock (HF) level is well controlled. However, the self-energy is divergent at the Fermi energy and it is not possible to define an effective mass. On the other hand, the logarithmic divergencies in the HF-free energy can be separated out and we are able to present a thermal effective mass at the HF level, viz., \( m^*_F \), arising entirely from exchange processes. Here we present previously unpublished results for the coefficients of the \( T^2 \) term of the polarized system. The HF \( m^*_F \) decreases with \( r_s \) and this approximation breaks down for \( r_s > 3 \) when \( m^*_F \) becomes negative. Thus the inclusion of correlation corrections is imperative to obtain a physically meaningful result.

Instead of using diagrammatic methods, in our previous work we used a calculation of \( F_{xc} \) at finite-\( T \) via a coupling-constant integration of the PDFs of the interacting system. The finite-\( T \) \( g(r) \) needed for the calculations were obtained using the classical-map hyper-netted-chain (CHNC) method where the 2D electron system at the temperature \( T = 0 \) is replaced by a classical Coulomb fluid at the temperature \( T_\eta \). Given that the interacting chemical potential \( \mu \) becomes negative beyond \( r_s \sim 2 \), (e.g., at \( r_s = 5 \), \( \mu/E_F \sim -5 \)), the distribution functions even at \( T \) just slightly above \( T = 0 \) are classical Boltzmann distributions with little or no occupation at \( k_F \). Hence the study of a classical model which correctly incorporates quantum features via effective potentials is a very reasonable proposition. However, although the CHNC can be unambiguously implemented at \( T = 0 \) and at sufficiently elevated temperatures, we are beset with a number of difficulties in dealing with the ‘warm-dense’ region close to \( T = 0 \). The two main difficulties are (a) the elimination of logarithmic-divergent terms which need to exactly cancel with the exchange and correlation contributions, (b) the finite-\( T \) modeling of the bridge function of the classical-fluid which controls the cluster diagrams beyond the hyper-netted-chain sum of diagrams. In this study we present an alternative approach which partially circumvents these difficulties, and provides a more transparent analysis, leading to a new formulation of the effective mass calculation.

The \( g(r_s,r) \), i.e., PDFs of the 2D-electron system (at \( T = 0 \)) have been accurately parametrized by Giri-Giorgi et al., [3] and may be considered known. The \( F_{xc} \) at \( T = 0 \) can be written as a coupling-constant integration over \( g(\lambda r_s,r) \) where \( \lambda \) is the coupling constant. Further more, we consider \( -\log\{g(r)\} \) as the potential of mean force, viz., \( \beta V_{mf}(r) \) of the equivalent classical interacting Coulomb fluid. Then we determine the finite-\( T \) form of \( \beta V_{mf}(r) \) to second order in the temperature and use this to directly evaluate the second-order temperature correction to the exchange-correlation free energy. In the following we show that the method leads to a transparent, if approximate, calculation of the effective mass \( m^* \) at arbitrary polarizations, and in good agreement with the available results in the field.

II. THEORY

The thermal effective mass \( m^* \) can be expressed as a ratio of the heat capacities of the interacting and non-interacting systems as:

\[
m^* = C_v/C_v^0 = \frac{\partial^2 F(T)/\partial T^2}{\partial^2 F_0(T)/\partial T^2}
\]

(1)

Here \( C_v \) is the specific heat at constant volume. The interacting free energy \( F \) is the sum \( F_0 + F_x + F_c \), where \( F_x \) and \( F_c \) are the exchange and correlation contributions, with \( F_{xc} = F_x + F_c \). Hence the problem of determining \( m^* \) reduces to a calculation of exchange-correlation effects at finite temperatures, near \( T = 0 \). However, such calculations are in many ways even more demanding than those at zero temperature, as perturbation methods have to now deal with a whole host of new diagrams, their singularities and cancellations. These difficulties were first addressed in the papers by Luttinger, Ward, and Kohn [2]. Similarly, QMC methods are also equally difficult, especially for \( T \) very close to zero.

The Hartree-Fock self-energy becomes logarithmically divergent near \( k_F \) and it is not possible to define an \( m^* \) via the self-energy at \( T = 0 \). In the following we first examine the exchange-only, i.e., Hartree-Fock, approximation to \( F \) at finite temperature, and calculate a regularized effective mass \( m^*_F = m_{HF} = 1 + \Delta m_z \) for paramagnetic and ferromagnetic 2D electrons, i.e., for spin polarizations \( \zeta = 0 \) and 1. It is found that \( m_z \), containing the corrections from \( F_{xc} \), is a decreasing linear function of \( r_s \) for both polarizations.
A. Non-interacting and Hartree-Fock Helmholtz free energies

The non-interacting free energy $F_0 = E_0 - TS$, where $S$ is the entropy, can be evaluated and expressed in terms of the dilogarithm function. Writing $\eta = \mu / T$, where $\mu$ is the chemical potential, $F_0$ and $E_0$ for the 2D system are given as follows, per unit atomic volume, and in Hartree atomic units:

$$E_0 = \frac{T^2}{2\pi} \left[ \frac{\pi^2}{6} + \frac{\eta^2}{2} + \text{dilog}\left(\frac{e^\eta}{1 + e^\eta}\right) \right] \quad (2)$$

$$F_0 = \mu n - \frac{T^2}{2\pi} \left[ \frac{\pi^2}{6} + \frac{\eta^2}{2} + \text{dilog}(1 + e^{-\eta}) \right] \quad (3)$$

Alternative expressions are possible, as given in ref. [4, 5]. The low-temperature expansion of $F_0(t)$ can be given as:

$$F_0(t, \zeta = 0) = E_0(0,0)(1 - 3.2859t^2) \quad (4)$$

$$F_0(t, \zeta = 1) = E_0(0,1)(1 - 0.82246t^2) \quad (5)$$

$$E_0(0, \zeta)/n = 0.5(1 + \zeta^2)/r_s^2 \quad (6)$$

The quadratic coefficient in the expansion of $F_0(t, \zeta)$ would be denoted by $a_2(\zeta)$ where needed. Thus $a_2(\zeta = 1) = -0.82246E_0$. Note that here we have used the same paramagnetic $E_F$ in defining $t = T / E_F$ for all 2D systems mentioned in the above equations.

The first-order (i.e., unscreened) exchange free energy $F_x$ consists of $F_x^1$, where $i$ runs over the two spin species. At $T = 0$ these reduce to the exchange energies:

$$E_x^i/n = -\frac{8}{3\sqrt{\pi}}n_i^{1/2} \quad (7)$$

Here $n_1 = n(1 + \zeta)/2$, and $n_2 = n(1 - \zeta)/2$. Then the exchange energy per particle at $T = 0$, i.e., the internal energy contribution $E_x/n$ at $T = 0$ becomes

$$E_x/n = (E_x^1 + E_x^2)/n = -\frac{8}{3\pi r_s} \left[ c_1^{3/2} + c_2^{3/2} \right] \quad (8)$$

Here $c_1$ and $c_2$ are the fractional compositions $(1 \pm \zeta)/2$ of the two spin species.

We also define the species-dependent reduced chemical potentials $\mu_i^0/T$ by $n_i$, reduced temperatures $t_1 = t/(1 + \zeta)$ and $t_2 = t/(1 - \zeta)$, based on the two Fermi energies $E_{F1}$ and $E_{F2}$ which are $E_F(1 \pm \zeta)$. Then we have:

$$F_x^i/E_x^i = \frac{3}{16} t_{1/2}^3 \int_{-\infty}^{n_i} \frac{I_{1/2}^2(u)}{(n_i - u)^{1/2}} du \quad (9)$$

The $I_{-1/2}$ is the Fermi integral defined as usual:

$$I_{\nu}(z) = \int_0^{\infty} \frac{du}{1 + e^{u}} \quad (10)$$

The $n_i$ are given by

$$n_i = \log(e^{1/t_i} - 1) \quad (11)$$

In the paramagnetic case Eq. (9) reduces to the result given by Isihara et al. [6] (see their Eqs. 3.4-3.6; they use a slightly different definition of the Fermi integral).

The total exchange free energy per unit atomic volume is $F_x = \Sigma F_x^i$. The accurate numerical evaluation of Eq. (9) requires the removal of the square-root singularity by adding and subtracting, e.g., $I_{1/2}^2(-|n|)/(v - |n|)^{1/2}$ for the case where $n$ is negative, and $v = u$, and so on.

A real-space formulation of $F_x = F_x^1 + F_x^2$ using the zeroth-order PDFs fits naturally with the approach of our study using pair-distribution functions of the electron fluid as the main ingredient. Thus

$$F_x/n = n \int \frac{2\pi r dr}{r} \sum_{i<j} h_0^{ij}(r) \quad (12)$$

Here $h_0^{ij}(r) = g_i^{ij}(r) - 1$. In the non-interacting system at temperature $T$, the antiparallel $h_{ij}^2$, viz., $g_{ij}^2(r, T) - 1$, is zero while

$$h_{11}^0(r) = -\frac{1}{n_i^2} \Sigma_{k_1, k_2} n(k_1)n(k_2)e^{(k_1-k_2)r} = -[f(r)]^2 \quad (13)$$

Here $k$, $r$ are 2-D vectors and $n(k)$ is the Fermi occupation number at the temperature $T$. At $T = 0$ $f(r) = 2J_1(kr)/kr$, where $J_1(x)$ is a Bessel function. As a numerical check, we have evaluated the exchange free energy by both methods, i.e., via $k$-space and $r$-space calculations.

The following small-$T$ expansions are useful for our purposes:

$$F_x(r_s, t, \zeta = 0) = E_x(r_s, \zeta = 0)[1 + (s^2/16)t^2\log(t) - 0.56736t^2 + \cdots] \quad (13)$$

This result, i.e., $F_x$ for the unpolarized system, has been given by Isihara et al. [6] and re-confirmed by Mahan et al. [7]. The corresponding internal energy, $E_x$, can be obtained from the relation $E = d[\delta F]/d\beta$ where $\beta = 1/T$. We refer to the coefficient of the $t^2\log(t)$ terms as $A_{L}$, and that of the quadratic term as $A_2$. These depend on the spin polarization $\zeta$. The results for the fully polarized case do not seem to be previously available in the literature. We have obtained the following expansion:

$$F_x(r_s, t, \zeta = 1) = E_x(r_s, \zeta = 1)[1 + (s^2/64)t^2\log(t) - 0.28368t^2 + \cdots] \quad (14)$$

B. The Hartree-Fock effective mass

The Hartree-Fock electron fluid is a theoretical construct which does not exist in nature. However, it is a very useful conceptual model. The difficulties in this conceptual model are due to the singular behaviour of the single-particle energy, self-energy etc., close to the Fermi energy. Thus taking derivatives near the Fermi energy becomes meaningless. However, as these divergences are
logarithmic, they can be integrated over and the free energy and related quantities can be evaluated. They are found to contain logarithmic terms which are explicitly exposed in Eqs. (13) and (14). These logarithmic terms, of the form $A_L(\zeta)t^2 \log(t)$ are removed when higher order corrections are included in the theory, while the quadratic term $A_2(\zeta)t^2$ contributes to the heat capacity. Hence it is clear that we can define a \textit{regularized} effective mass by dropping the $t^2 \log(t)$ terms and calculating an $m_x$ entirely from the coefficient $A_2$. Thus

$$m_x(\zeta) = 1 + A_2(\zeta)/a_2(\zeta)$$

(15)

Here $a_2$ is the coefficient defined in Eq. (4) in the expansion of $F_0$. Results from such calculations are shown in Fig. 1. These results show how the exchange contributions widen the Hartree bandwidth with the decrease of the effective mass. For $r_s > \sim 3$, the value of $m^*$ becomes negative. Clearly, the Hartree-Fock model is misleading except at smaller $r_s$.

III. CORRELATION CORRECTIONS TO THE FREE ENERGY AND THE EFFECTIVE MASS.

Microscopic theories of Landau Fermi liquids calculate $m^*$ from the solutions of the Dyson equation for the one-particle interacting Green’s function of the system. If the real part of the retarded self-energy is $\Sigma_\text{r}(\vec{k}, \omega)$, the Landau quasi-particle excitation energy $E_{QP}(\vec{k})$, measured with respect to the chemical potential is used in calculating the effective mass $m^*$.

$$E_{QP}(\vec{k}) = \epsilon_k + \Sigma_\text{r}(\vec{k}, \omega)|_{\omega = E_{QP}}$$

(16)

$$\epsilon_k = k^2/2 - E_F$$

(17)

$$\frac{1}{m^*} = \frac{dE_{QP}(k)}{dk}|_{k=k_F}$$

(18)

The quasiparticle energy is the eigenvalue of the Dyson equation and contains the non-interacting energy $\epsilon(k)$ plus the real part of the the selfenergy $\Sigma(k, \omega)$ evaluated self-consistently at the quasiparticle energy itself. We may rewrite the selfenergy as an exchange part, and a correlation contribution:

$$\Sigma = \Sigma_x(k) + \Sigma_c(k, \omega).$$

(19)

This should be evaluated self-consistently to satisfy sum rules, Ward identities etc., to give a conserving approximation. In practice, these self-consistency conditions have to be stringently satisfied if the logarithmic singularities in $\Sigma_x$ are to be completely cancelled by corresponding singular terms contained in $\Sigma_c$. Thus any approximate theory must necessarily be on guard against spurious contamination from inadequate cancellations. These could greatly enhance the calculated $m^*$, as is indeed observed in some RPA-type calculations. Further more, the interacting chemical potential $\mu/E_F$ is very different from unity, and strongly negative. These may be avoided in the attempt to impose self-consistency a very daunting task. In the temperature theory, say Eq. (13) of the previous subsection, these would manifest as spurious contributions to $m^*$ proportional to $1/t$ as $t \to 0$.

The exchange and correlation free energy $F_{xc}(r_s, t)$ at any temperature and spin-polarization can be evaluated from pair-distributions functions rather than from self-energies or Green’s functions. The exchange free energy $F_x$ is just the contribution to a coupling constant integration (see below) over the PDFs at zero coupling (see Eq. (12)). The $F_x$, evaluated from the non-interaction PDF, $g_0(r)$ via Eq. (12) contains singular logarithmic terms. These singular terms at zero coupling are offset by the contributions from the rest of the coupling-constant integration reaching out to full coupling.

$$F_{xc}(r_s, t)/n = \int_0^1 d\lambda \int \frac{2\pi r dr}{r} \sum_{ij} c_i c_j(g_{ij}(r, \lambda) - 1)$$

(20)

Here $\lambda$ is the coupling constant. The $r_s$, and $t = T/E_F$ dependences in the $g_{ij}(\lambda, r)$ are not displaced for brevity. In our previous work (e.g., ref. [8] and references there-in) the needed $g_{ij}(r)$ are calculated at any given temperature $T$ (including $T = 0$) using the CHNC method for 2D systems [8, 9]. In CHNC, the quantum fluid at $T = 0$ is replaced by a classical fluid at $T_\text{Q} = 1/\beta$. At finite temperatures $T > 0$, $\beta = 1/\sqrt{T^2 + T^2}$. Although this method gave reasonable results for $m^*$ via Eq. (1) the question

FIG. 1: The panel (a) shows the modification of the chemical potential $\mu$ due to interactions, driving it to the negative regime for $r_s > \sim 1$. Negative $\mu$ is typical of classical fluids. (b) The Hartree-Fock effective mass, $m^*_x$, is shown as a function of the density parameter $r_s$, for the polarizations $\zeta = 0$ and 1.
of the extension of model bridge functions to finite-$T$, as well as the accuracy of the cancellation of logarithmic terms which should cancel accurately remained troubling issues. Numerical calculations very close to $T = 0$ are also very susceptible to difficulties due to the sharpness of the Fermi functions at very low $T$.

Accurate pair-distribution functions of the 2D-UEF at $T = 0$ are now available from QMC as well as from analytical representations developed by Gori-Giorgi et al. We use these functions instead of those generated from the CHNC, as this is equivalent to replacing the hard-disk bridge functions of the CHNC description with the Coulomb bridge function [3]. If the 2D-PDF, i.e., $g(r)$, obtained by these methods were that of a classical fluid, then it would be of the form:

$$ g(r) \mapsto \exp[-\beta V_{mf}(r)] \quad (21) $$

$V_{mf}(r)$ is known as the potential of mean force, and is simply the Kohn-Sham potential at $r$ in a classical fluid where one particle is already at the origin. The CHNC attempts to construct $\beta V_{mf}(r)$ directly from the diffraction-corrected Coulomb potential $V_{dc}(r)$ and the Pauli-exclusion potential $P(r)$ via the modified HNC equation. These potentials are discussed in greater detail in refs. [4, 5].

$$ g(r) = \exp[-\beta V_{dc}(r) - \beta P(r) + N(r) + B(r)] \quad (22) $$

Here $N(r)$ is known as the nodal function, while $B(r)$ is the bridge functions [10] which bring in multi-particle clustering effects which are outside the scope of the hyper-netted-chain diagrams. The potentials $V_{dc}(r)$, and $P(r)$ are long-ranged, while $N(r), B(r)$ contain many-body effects, and screening effects which damp $V_{dc}(r), P(r)$, so that $g(r) \to 1$ for large $r$.

In the present study we follow a different strategy. The potential of mean force, $\beta V_{mf}(r, T)$ at finite-$T$ is developed as a Taylor expansion around $T = 0$, i.e., around $\beta = 1/T_q$ and $F_{xc}$ is calculated using the $T = 0$ PDF.

$$ \beta = 1/(T_q^2 + T)^{1/2} \quad (23) $$

$$ \beta V_{mf}(r, T) = \beta V_{mf}(r, 0) + (T^2/2) \frac{\partial^2 \beta V_{mf}(r, T)}{\partial T^2} \bigg|_{T=0} \quad (24) $$

$$ F_{xc}(T)/n = F_{xc}(T = 0)/n + (T^2/2) \Delta F_{xc} \quad (25) $$

$$ \Delta F_{xc} = (T^2/2) \int_0^1 d\lambda n \int_{-\infty}^{\infty} \frac{2\pi r dr \Gamma(r, T, \lambda)}{r} \quad (26) $$

The effect of the nodal term $N(r)$ and the bridge term of Eq. (22) is simplified and subsumed in the screening wavevector $k_{sc}$. At high densities, i.e., $r_s \leq 1$, electrostatic potentials screen at the Thomas-Fermi value $2m/E_F = 2$, and drop to about half this value at low densities. This is further discussed in the section on results, given below. Also, the $T$-dependence or polarization dependence in the screening parameter is neglected in the present study.

The diffraction corrected Coulomb potential and the Pauli exclusion potential are of the form

$$ V_{dc} = (1/r) \{ 1 - e^{-k_{sc}r} \} \quad (27) $$

The de Broglie thermal wave vector $k_{th} = \{ \pi T_q \}^{1/2}$ at $T = 0$ appears in $V_{dc}(r)$. Its temperature dependence is neglected in our context as it only modifies the very small-$r$ region, where $g(r)$ is negligible. Hence it plays no significant role in Eq. (23) The Pauli exclusion potential $\beta P(r)$ is given by

$$ \beta P(r) \delta_{ss'} = -\log(g^0(r)) + (g^0(r) - 1) + \beta^0(r) \quad (28) $$

Here $\beta^0(r)$ denotes the ‘direct-correlation function’ of Ornstein-Zernike theory. It can be calculated from $g^0(r)$, i.e., the non-interacting pair-distribution function for parallel spins $s = s'$. An average potential may also be defined for use with the paramagnetic system treated as a single species, using $g^0_{\pi r_1} = 0.5(g^0_{11} + g^0_{12})$ in Eq. (28). Hence $P(r)$ is known at any temperature and $r_s$. It is a universal function of $r/r_s$, and known only as the product of $\beta$ and $P$. However, we may use the CHNC values of $T_q$ to define a $\beta$ at any $r_s$ and determine $P(r)$ by itself. We have numerically calculated its second-order temperature derivative (Fig. 2) and denote it as $\beta^{(2)} P(r)$ in the following. These quantities are now assembled together to calculate the second-order finite-$T$ correction to $F_{xc}$. We have:

$$ \Gamma(r, T, \lambda) = \Gamma(mf) + \Gamma(P) \quad (29) $$

$$ \Gamma(mf) = \sum_{ij} c_i c_j \frac{\partial \beta V_{mf}(r, 0)}{\partial T_q} \quad (30) $$

$$ \Gamma(P) = - \sum_{ij} c_i c_j \frac{\partial \beta P^{(2)}(r, 0)}{\partial T_q} \delta_{ij} |_{T=0} \quad (31) $$

$$ m^*(\zeta) = 1 + \Delta F_{xc}(\zeta)/\alpha_2(\zeta) \quad (32) $$

The $m^*(\zeta)$ coefficient in the last equation is the coefficient of the $T^2$ term in the interacting free energy, as in Eq. (1). The first term in the r.h.s. of Eq. (29) arises from the temperature derivative of $\beta$ in $\beta V_{mf}(r, T)$, evaluated at $T = 0$, while the second term is from the second temperature derivative of the Pauli exclusion potential. In evaluating Eq. (29) we use the pair-distribution functions of Giri-Giorgi et al. [8], as the approximate forms derived from CHNC using a hard-disk bridge function are less accurate. The 2D quantum temperature $T_q$ and other CHNC procedures used here are those given by Perrot and Dharma-wardana in ref. [5].
FIG. 2: The Pauli exclusion potential $\beta P(r)$ for 2D-electrons, and its second temperature derivative ($t = T/E_F$), derived from $g_0^0(r)$. The bottom panel shows the results for the paramagnetic, i.e., averaged $g^0(r)$. These potentials exactly reproduce the Fermi hole in the pair-distribution functions.

Eq. 29 provides a new model for the calculation of the effective mass $m^*$ as a sum of contributions from the temperature dependence of the potential of mean force, $m_{xc}(mf)$, and the temperature dependence of the Pauli-exclusion potential, $m_{xc}(P)$. These contributions are shown in Figs. 3 and 4 and labeled according to the following equation.

$$m^* = 1 + m_{xc} = 1 + m_{xc}(mf) + m_{xc}(P)$$

$$m^* = m(mf, P); \quad m^*(mf) = 1 + m_{xc}(mf)$$

The contribution $m_{xc}(mf)$ may be thought of as resulting from temperature dependent modifications in exchange-correlation contributions as a function of $r_s$ due to screening, while $m(P)$ are contributions from the screened exchange interactions. Only the second-order temperature derivatives have been used as the first-order derivatives (which contain logarithmic terms of the form $t^2\log(t)$) are considered to cancel themselves out in an accurate theory.

The essential weak point of this calculation is in the specifying of the screening factor $k_{sc}$ in Eq. 26. A one-parameter screening approach is indeed very approxi-
This work $m^*(mf)$
QMC Drummond-Needs Expt., Padmanabhan et al.
GW-SC Asgari et al
GW-OSA Asgari et al.

FIG. 4: The effective mass $m^*$ as a function of the density parameter $r_s$, for polarized ($\zeta=1$) 2D electrons. See text for more details.

mate. However, this is guided by our calculation of $m^*(mf)$ shown in Fig.s 3 and 4. While the high-density Thomas-Fermi $k_{sc}$ is 2 for electrostatic interactions, we have used 2.5 for $r_s$ below unity for the screening of the exchange interactions brought in by the Pauli potential. The screening parameter $k_{sc}$ drops to 2 at $r_s = 4$, then to 1.54 at $r_s = 10$, and unity near $r_s = 30$. By $r_s = 30$, $m^*$ becomes 1.34 for $\zeta=0$, and takes the value of 0.817 for $\zeta = 1$. Drummond and Needs have recently reported a QMC value of $m^* = 1.34$ at $r_s = 10$ for $\zeta = 0$. Our model does not exclude such higher values of $m^*$, but this would require a significantly weaker screening of the potentials, which accommodates less comfortably with the behaviour of the potential of mean force (eq. [21] as a function of $r_s$.

V. CONCLUSION

We have presented results for the effective mass $m^*$ as a function of the density and polarization of a 2-D electron fluid, using an entirely new approach based on the known pair-distribution functions of the 2D fluid. Good agreement with the trends and magnitudes observed in recent experimental and theoretical approaches to the problem are recovered. The essential inputs to the present calculation are: (i) the pair distribution functions of the 2D-electron fluid as parametrized by Gori-Giorgi et al [3], (ii) the Pauli exclusion potential extracted from the non-interacting PDF, (iii) elementary thermal physics, and (iv) some classical-map HNC concepts from the theory of classical statistical mechanics. The method provides a physical understanding of the processes contributing to the enhancement or diminution of the effective mass.

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