Layer-thickness effects in quai-two dimensional electron liquids.

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We use a mapping of the quasi-2D electron liquid to a classical fluid and use the hypernetted-chain equation inclusive of bridge corrections, i.e., CHNC, to calculate the electron pair-distribution functions and exchange-correlation energies as a function of the density, layer width, spin-polarization and temperature. The theory is free of adjustable parameters and is in good accord with recent effective-mass and spin-susceptibility results for HIGFET 2-D layers.

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The 2-D electron systems (2DES) present in GaAs or Si/SiO$_2$ nanostructures access a wide range of electron densities under controlled conditions, providing a wealth of information which is of basic and technological importance. The 2DES is in the x-y plane and also has a transverse extension in the lowest sub-band of the hetero-structure. The higher subbands are far above the Fermi energy and no upward excitations are possible. Although the z-motion is confined to the lowest subband, realistic layers may have widths of $\sim 600 \text{Å}$ or more, and this corresponds to $\sim 6$ effective atomic units in GaAs. Recent experiments and theory have focused on these layer-thickness effects [6, 7, 9, 10, 11]. The physics of the layer thickness effects depends on the density parameter $\nu$, and the temperature $T$. The 2D density $n$ defines the mean-disk radius $r_s = (\pi n)^{-1/2}$ per electron, expressed in effective atomic units which depend on the bandstructure mass $m_b$ and the “background” dielectric constant $\varepsilon_b$. Although $r_s$ is the “small parameter” in perturbation theory (PT), here it is simply the electron-disk radius and PT is not used.

Finite-width effects of the 2DES arise also in the quantum Hall effect, where an “unperturbed-$$q$$” approximation, which uses the pair-distribution function (PDF) of the ideal 2DES and the quasi-Coulomb potential $W(r)$ of the thick 2D layer are used to calculate energies.

While diagrammatic methods propose “turn-key” procedures for calculating many-body properties, they work only for weakly coupled (small $r_s$) systems, where RPA-like approximations may be used. Variied results can be obtained using various approximations which go “beyond” RPA. Unfortunately, an approximation successful with one property usually fails for other properties. Such methods lead to negative PDFs, incorrect local-field corrections in the response functions, and disagreement with the compressibility sum rule etc., and incorrect predictions of spin-phase transitions (SPT) at quite high densities. In fact, alternative approaches were sought by Singwi, Tosi et al. (STLS) [12], and Ichimaru et al. [13], and also within the Feenberg-type correlated-wavefunction methods [14]. Most of the currently available results for strongly-coupled systems have been generated using correlated-wavefunction approaches via Quantum Monte Carlo (QMC) simulations. However, QMC remains a strongly computer-intensive numerical method which is best suited for the study of simple “bench-mark” systems.

We have recently introduced a conceptually and numerically simple, adequately accurate method for strongly-correlated quantum systems at zero and finite temperatures, where the objective is to work with the PDF of the quantum fluid, generated from a classical Coulomb fluid whose temperature $T_q$ is chosen to reproduce the correlation energy of the original quantum fluid at $T = 0$. The classical PDFs are obtained from an integral equation equivalent to a classical Kohn-Sham equation where the correlation effects are captured as a sum of hyper-netted-chain (HNC) diagrams and bridge diagrams. This method, known as a Classical mapping to an HNC form, i.e, CHNC, was applied to the 3D and 2D electron fluids [15, 16, 17, 18], to dense hydrogen fluid [19], and also to the two-valley system in Si-MOSTFETS [20, 21]. In each case we showed that the PDFs, energies, etc., obtained from CHNC were in excellent agreement with comparable QMC results [21, 22]. Variants of the method have also been discussed by Bulutay and Tanatar, and by Khanh and Totsuji [23].

The advantage of CHNC is that it affords a simple, semi-analytic theory for strongly correlated systems where QMC becomes prohibitive or technically impossible to carry out. The classical-fluid model allows for physically motivated treatments of complex issues like three-body clustering etc., via the statistical mechanics of hard-disk reference fluids [20]. The disadvantage of the method, typical of such many-body approaches, is that it is currently an “extrapolation” method taking off from the results of a model fluid. For 2D systems, the fully spin-polarized ideally-thin uniform fluid is the model fluid [17]. As the CHNC method has been
described in previous work, we do not give a detailed account here. This study is a simple, direct application of CHNC to the quasi-2D potential \( W(r) = V(r)F(r) \), where \( V(r) = 1/r \) and \( F(r) \) is a form-factor accounting for the modifications arising from the thickness effect.

Most of our calculations are for the Fang-Howard (FH) approximation\(^2\) to the charge density \( n(z) \) contained in HIGFET structures of the type used by Zhu et al.\(^5\). In this case, \( F(k) \), the form factor in \( k \)-space, has an analytic form but \( F(r) \) is numerically determined. It is technically convenient to work with an equivalent constant-density model (CDM) for which analytic forms are available for \( F(r) \) as well as \( F(k) \). We present a potential \( W(r, w) \) for a CDM which is *electrostatically equivalent* to the 2D potential for any \( n(z) \), e.g., the FH-potential defined by the parameter \( b \). The method of replacing an inhomogeneous distribution by a uniform distribution is suggested by the observation that the non-interacting total correlation function \( h^0(r) = g^0(r) - 1 \) has the form \( \sim n(r)^2 \), where \( n(r) \) is the density-profile around the Fermi hole. We replace the inhomogeneous \( n(z) \) by a slab of constant-density \( n_{cd} \) which is easily shown to accurately recover the electrostatic potential of \( n(z) \) in the 2-D plane.

\[
n_{cd} = 1/w = \int n(z)^2 dz \quad (1)
\]

Since the subband distribution is normalized to unity, the width \( w \) of the CDM is simply \( 1/n_{cd} \). Hence quasi-2D layers can be labeled by their effective width \( w \). The CDM width \( w \) for the \( n(z) \) labeled by the Fang-Howard \( b \) is \( w = 16/(3b) \), and differs from the commonly quoted “thickness” \( 3/b \). This provides an explicit example of the replacement of an inhomogeneous distribution by a homogeneous distribution, already suggested in Ref.\(^{27}\) and used for 2-electron atoms. The quasi-2D potential for a CDM of width \( w \) is given by

\[
W(r) = V(r)F(s), \quad s = r/w, \quad t = \sqrt{1 + s^2} \\
F(r) = 2s[\log(s/t) + t] \quad (2)
\]

This tends to \( 1/r \) for large \( r \). The short-range behaviour is logarithmic and weaker than the \( 1/r \) potential. The form factor \( F(r) \) for a HIGFET with \( r_s = 5 \) is shown in the inset to Fig.\(^{[1]}\). The \( k \)-space form of the CDM potential is:

\[
W(k, w) = V(k)F(p), \quad p = kw \quad (3) \\
F(p) = (2/p)\{(e^{-p} - 1)/p + 1\} \quad (4)
\]

The form factors \( F(s) \) and \( F(p) \) tend to unity as \( w \to 0 \). These \( r \)-space and \( k \)-space analytic forms of the CDM indirectly lead to analytic formulae for the FH from. The \( W(r) \) of the CDM is equivalent to that from the original inhomogeneous distribution, and only \( W(r) \) enters into the exchange-correlation and \( g(r) \) calculations.

In the case of GaAs-HIGFETS, if the depletion density could be neglected, \( r_s \) specifies the \( b \) parameter and hence the width \( w \) of the CDM. Then \( b^3 = 33/(2r_s^2) \) and \( w = 2.09494r_s^{2/3} \). When the exchange-correlation energy \( E_{xc}(b, r_s) \) is included, \( b \) changes to \( b^* \). The correction is \( \sim 2 - 3\% \) at low \( r_s \to 1 \) and decreases as \( r_s \) increases. We have used \( b^* \) in our fully self-consistent CHNC calculations.

**Exchange and correlation in quasi-2D layers.**— The noninteracting-2D correlation function, \( h^0(r) = g^0(r) - 1 \), yields exact exchange energies for arbitrary \( w \) as well as for \( w = 0 \) (the ideal 2DES). On the other hand, the correlation-energy evaluation needs the PDFs of the quasi-2D potential \( \lambda W(r, w) \), at many values of the coupling constant \( \lambda \). These \( g(r, \zeta, w, \lambda) \) can be calculated using the CHNC. However, the use of the *unperturbed-g* approximation used in Quantum Hall studies\(^{[4]}\) can be useful here too. De Palo et al.\(^{[8]}\) have in fact exploited

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**FIG. 1:** (a) The effective mass \( m^* \) of an ideal 2D layer (\( w = 0 \)) obtained here are compared with the the QMC data of Ref.\(^{[31]}\) and the \( G_{i+k}G_{-i}/D \) calculation of Asgari et al.\(^{[10]}\). (b) The effective mass \( m_{ch}^* \) in a HIGFET using the CHNC ideal-2D finite-\( T \) \( g(r) \) in the “unperturbed-\( g \)” approximation, i.e., Eq.\(^{[5]}\). The HIGFET calculation of Asgari et al. is also shown.
such an approach where the \( g(r, \zeta, w = 0) \) of the ideally thin layer are used to calculate a correction energy \( \Delta \) given by,

\[
\Delta = (n/2) \int 2\pi r dr [W(r) - V(r)] h(r, \zeta, w = 0) \quad (5)
\]

Then the total \( E_{xc}(r_{s}, \zeta, w) \) is obtained by adding to \( \Delta \) the known \( E_{xc} \) of the ideally-thin system. The “unperturbed” \( g(r) \) needed in Eq. 5 at \( T = 0 \) are the QMC \( g(r) \) [3]. Equation 5 can also be applied to the finite- \( T \) ideal \( g(r_{s}, \zeta, T) \) obtainable from CHNC. However, this approach is found to be insufficient for calculating \( m^{*} \).

De Palo et al. have performed Diffusion Monte Carlo simulations at \( r_{s} = 5 \) for HIGFETS with \( b = 0.8707 \), i.e., a CDM width \( w = 6.1256 \) a.u., and find that the error compared to the full simulation is about 2%. Since the ratio \( w/r_{s} \) decreases in the HIGFET as \( r_{s} \) increases, the HIGFET approaches the thin-layer model for large \( r_{s} \). Hence Eq. 5 is satisfactory for \( r_{s} \geq 5 \), and unreliable for small \( r_{s} \), e.g., below \( r_{s} = 3 \). Equation 5 neglects the renormalization of the kinetic energy, correction of \( b \) to \( b^{*} \), as well as the changes in \( g(r) \) due to the changed potential. We have used both the full CHNC which accounts for all these effects, and also the “unperturbed- \( g \)” approximation, Eq. 5, and find that the latter is indeed satisfactory for the calculation of \( E_{xc} \) and the susceptibility enhancement \( m^{*} g^{*} = \chi_{s}/\chi_{p} \), where \( \chi_{s} \), \( \chi_{p} \) are the interacting and Pauli spin susceptibilities.

**Correlation energy at finite temperatures.**— The correlation contribution to the Helmoltz free energy of ideal \( (w = 0) \) or thick layers \( (w > 0) \) is readily calculated via Eq. 5 using the CHNC-finite- \( T \) \( g(r) \). For example, consider \( r_{s} = 5 \), and \( T/E_{F} = 0.05 \), with \( \eta = 0.3718 \), i.e., the packing fraction of the hard-disk fluid used to mimic the three-body terms in the extended HNC equation. Then \( E_{xc} \) for the ideal 2D at \( \zeta = 0 \) is \(-0.16902 \) a.u., while the HIGFET \( E_{xc} \) from Eq. 5 and from the full CHNC are \(-0.11197 \) a.u. and \(-0.11467 \) a.u. respectively. As discussed in earlier work [21, 22], the exchange free energy \( F_{x} \) and the correlation free energy \( F_{c} \) at very low \( T \) contain logarithmic terms which cancel with each other, so that the sum \( F_{xc} = F_{x} + F_{c} \) free of such terms. At \( r_{s} = 5 \) the cancellation is good to about 75%, and this improves as \( r_{s} \) increases. Although the two-component fluid (up and down spins) involves three distribution functions, we have, as before [17], used only one hard-disk bridge function, \( B_{12} \), as clustering effects in \( g_{ii} \) are mostly suppressed by the Pauli-exclusion. This is a satisfactory approximation for \( r_{s} \geq 3 \), and for smaller \( r_{s} \) \( B_{12} \) becomes comparable to \( B_{ii} \), but negligible. Also, \( B_{12} \) is assumed to be independent of \( \zeta \) and identical to the ideal-2D \((w = 0)\) bridge function.

The **spin-susceptibility, \( m^{*} \) and \( g^{*} \)**.— The results for the \( F_{xc}(r_{s}, \zeta, T, w) \) of the ideal or thick 2DES suffice to calculate the spin-susceptibility enhancement, the effective mass \( m^{*} \) and the effective Landé factor \( g^{*} \). We calculate the quantity \( A = 1 + B(x) \), where \( B(x) \) is the ratio of the second derivative with respect to \( x \) of \( F_{xc}(x) \), and \( F_{0}(x) \), where \( x = \zeta \) for the spin susceptibility calculation, and \( x = T \) for the \( m^{*} \) calculation. \( F_{0}(x) \) is the noninteracting Helmholtz free energy. The CHNC is used to obtain any data (e.g., at finite - \( T \)) unavailable from QMC. The effective mass \( m^{*}_{H} \) obtained for the HIGFET using Eq. 5 where the ideal 2D-finite- \( T \) \( g(r) \) is used, is presented in the lower panel of Fig. 1. The upper panel shows the ideal 2D-layer \( m^{*} \) in good agreement with the four QMC values. This contrasts the \( m^{*} \) proposed by Asgari et al, denoted \( G_{+} & G_{-}/D \) in their paper [10]. A study of the local-field factor of the 2D response function [21] shows that the formation of singlet-pair correlations is complete by \( r_{s} \sim 5 \), and after that the structure of the fluid remains more or less unchanged, until the spin-phase transition (SPT) is reached. The rapid rise in \( m^{*} \) before \( r_{s} \sim 5 \) and the subsequent slow-down are probably related to the formation and persistence of singlet structure in the 2D fluid.
HIGFET, where as Asgari et al. predict the opposite. 

mal[9] have calculated work as well as for the thicker 2DES in they obtain close agreement with the data for very nar-

The weakened repulsion in the fully self-consistent g(r) are also shown in the inset, and shows a deviation of ~ 5%. This deviation is probably a short-coming of the CHNC model, associated with the use of a spin-independent bridge function.

The effective Landé-g factor.— The agreement between the experimental χs/χP ratio (i.e., m∗g∗) and the theoretical results, especially those from QMC for the ideal 2DES and the HIGFET suggests that m∗g∗ is known with some confidence. Hence we may extract the effective Landé-g factors for the ideal 2DES and the HIGFET (see Fig. 3), using the available m∗ values. The strong increase in m∗ with rs in HIGFETS implies that the g∗-factor is less sensitive to rs. This is similar to the behaviour of the two-valley system found in Si-MOSFETS where there is no SPT[21,22]. The additional inter-valley Coulomb interactions in MOSFETS weakens the role of exchange and enhanced the effect of singlet-pair cluster effects, leading to a strong increase around rs = 5. In the HIGFET, the the weakening of the repulsive interaction increases clustering, and boosts m∗, since quasi-particles no longer move freely, but have to drag a cloud of electrons associated with the enhanced g(r) near r/r∗ → 0. This shows that the m∗ calculation is very sensitive to the accurate evaluation of the “on-top” value of g(r = 0). In the CHNC, clustering and such effects are controlled by the hard-disk bridge function, and the diffraction correction (de Broglie momentum kth) used to describe the quantum-scattering of two electrons. In this work we have simply used the η and kth of the ideal 2DES, i.e., w = 0. Better agreement of m∗ with experiment would require an evaluation of these as a function of w. Similarly, complete QMC runs for finite w would require back-flow and three-body functions different from the usual RPA-like treatment of the 2DES.

Conclusion— We have used a single theoretical framework, i.e., the CHNC, with no parameters other than those previously used for the ideal 2D system[17], to calculate the Fxc(rs,ζ,T,w), and hence the m∗ and g∗ of thick 2D layers. The results suggest that the enhanced mass in HIGFETS arises from the strong short-range correlations created by the weakened Coulomb repulsion due to the thickness effect.

FIG. 3: The Landé g-factor for the ideal 2D Layer is obtained from the QMC m∗g∗ of ref. [32], divided by the CHNC ideal 2D m∗. The experimental HIGFET gH∗(boxes) is from the m∗g∗ of Zhu et al., divided by the m∗ of Tan et al. We also show gH∗ calculated from the m∗g∗ and the mH∗ results for the HIGFET. The inset shows the spin-susceptibility enhancement m∗g∗ from the ζ dependent energies calculated from Eq. 3 where the ideal 2D g(r) is used, and from the full CHNC calculation using the g(r) consistent with the quasi-2D potential.

In the lower panel of Fig. 1 we present the effective mass mH∗ of the electrons in the HIGFET. The “unperturbed-g” model, Eq. 5, is unable to approach the experimental results (Fig. 2) of Tan et al. Hence we repeat the m∗ calculations using the fully self-consistent g(r) from CHNC. The g(r) for the ideal 2DES and the fully self-consistent g(r) for a HIGFET at rs = 5, T/EF = 0.1 are shown in the upper panel of Fig. 2. The weakened repulsion in W(r) for small-r in the quasi-2DES allows easier electron clustering, strongly boosting the g(r) near r = 0. The HIGFET m∗, evaluated from the second derivative of Fxc(T) in the range T/EF = 0.05 to 0.1, is shown in the lower panel. Note that m∗ in our work increases from the ideal (w = 0) system to the HIGFET, where as Asgari et al. predict the opposite.

Enhancement of the spin susceptibility. De Palo et al.[16] have calculated m∗g∗ from the ideal QMC g(r), using the “unperturbed-g” approximation, and shown that they obtain close agreement with the data for very narrow 2-D systems[32] as well as for the thicker 2DES in HIGFETS[8], as shown in the inset to Fig. 3. We obtain results in close agreement when the “unperturbed-g” approximation, Eq. 5, is used. The m∗g∗ from the fully self-consistent g(r) are also shown in the inset, and shows a deviation of ~ 5%. This deviation is probably a short-coming of the CHNC model, associated with the use of a spin-independent bridge function.

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