The effective mass and the $g$-factor of the strongly-correlated 2-D electron fluid. Evidence for a coupled-valley state in the Si system.

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Abstract. – The effective mass $m^*$, and the Landé $g$-factor of the uniform 2-D electron system (2DES) are calculated as a function of the spin polarization $\zeta$, and the density parameter $r_s$, using a non-perturbative analytic approach. Our theory is in good accord with the susceptibility data for the simple 2DES, and in excellent agreement with the two-valley Si-2DES data of Shashkin et al. While $g^*$ is enhanced in GaAs, $m^*$ is enhanced in Si. The two-valley susceptibility is treated within a coupled-mode (coupled-valley) approach. The coupled-valley model is confirmed by comparison with the Quantum Monte Carlo results for a 4-component 2DES.

The 2-D electron fluid (2DES) exhibits a wealth of intriguing physics, straddling a rich phase diagram [1,2]. The phase diagram contains spin-polarized states at sufficiently large $r_s$, say $\sim 20 - 27$. Here $r_s = (\pi n)^{-1/2}$ is the electron-disk radius [3,4] at the density $n$, in atomic units. It is also equal to the value of the coupling constant $\Gamma = (\text{potential energy})/(\text{kinetic energy})$. The intermediate regime $r_s \sim 5 - 20$ also hosts many ill-understood phenomena including the metal-insulator transition (MIT) [5]. Anomalous values (e.g., see [6]), of $g^*$ and $m^*$ have been found. Some experiments suggest that an enhancement of $g^*$ is responsible for the strong enhancement of $m^* g^*$, while results [7] on Si metal-oxide field effect transistors (MOSFETs) suggest that it is $m^*$, and not $g^*$ which is enhanced. In this study we show that, for ideally thin 2-D layers, $g^*$ is enhanced in GaAs-like systems, while $m^*$ is enhanced in Si-like multi-valley systems. The existence of a coupled-valley state follows naturally from the physics of the Si system, and here we present a model leading to excellent quantitative agreement with experiment, and with Quantum Monte Carlo (QMC) simulations of a 4-component 2DES [8].

Fermi liquid-type theories [9] are valid for $r_s < 1$. Such perturbative methods have been applied, invoking impurities [10], or charge and spin-density wave effects [11]. On the other hand, QMC calculations of $m^*$ involve the excited states of the 2DES and are less reliable than for the ground state. QMC results up to $r_s = 5$ have been reported [12].

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We showed recently that the 2-DES, 3-DES, and dense hydrogen can be studied using a mapping to a classical fluid [13–16]. The accuracy of the map was established by comparison with QMC and other independent calculations. Here we use this classical map to evaluate \( m^* \) and \( g^* \) for the low-density 2-DES. The method is best understood within a density-functional picture.

The density-functional perspective. The Hohenberg-Kohn-Mermin theorem asserts that the Helmholtz free energy \( F \) is a minimum at the true density [17]. If \( n(r) \) is the true density, it obeys the variational equation \( \delta F[n(r)]/\delta n(r) = 0 \). If the origin of coordinates is on an electron, then if \( n(r) \) is the density as seen from this electron, it is a pair-density such that \( n(r) = n g(r) \). Here \( g(r) \) is the electron-pair distribution function (PDF). The variational condition gives the Kohn-Sham (KS) equation as usual. Then \( n(r) \) is obtained via a sum over the KS orbital-densities \( |\psi_i|^2 \) weighted by the Fermi factors \( f_i \). If the electrons formed a classical system, the variational equation becomes the Boltzmann form for the density:

\[
n(r) = ne^{-\beta(V_{\text{coul}}(r)+V_p(r)+V_c(r))}.
\]  

(1)

\( V_{\text{coul}}(r) \) is the Coulomb interaction between the electron at the origin and the electron located at \( r \). Similarly, \( V_p(r) \) is the Poisson potential at \( r \), and \( V_c(r) \) is a correlation potential. For a classical system the \( V_{xc}(r) \) of standard KS theory is replaced by just a correlation potential \( V_c(r) \). In effect, Eq. (1) evaluates the \( g(r) \) of the classical fluid. However, the \( g(r) \) of a classical fluid is accurately given by the hyper-netted chain (HNC) inclusive of a bridge function [18]. Thus, the extended HNC equation is a classical KS equation where \( V_c(r) \) is the sum of HNC+bridge diagrams. The construction of the Bridge diagrams for the 2DES is given in refs. [15, 20].

The classical map has no exchange, and fails as \( T \to 0 \). We rectify these lacunae as follows. In a system without Coulomb interactions, \( g(r) \) should reduce to \( g^0(r) \) which is known analytically (at \( T = 0 \)) or numerically. The first step of the mapping is to introduce a potential \( \phi_{ij}^0(r) \) (where \( i, j \) are spin labels) such that \( \phi_{ij}^0(r) \) generates \( g^0_{ij}(r) \) when used in the HNC equation for ideal electrons [19]. This leads to an exact treatment of exchange.

Electrons at \( T = 0 \) have kinetic energy. Hence the classical map of the quantum fluid at \( T = 0 \) would be at some “quantum temperature” \( T_q \). This is determined by requiring the correlation energy \( \epsilon_c \) of the classical fluid at \( T_q \) be equal to the \( \epsilon_c \) of the quantum fluid at \( T = 0 \). This may be regarded as a “calibration” of the classical fluid to recover the quantum exchange-correlation energy in the \( r_s \) range of interest. Here we use the \( \epsilon_c(r_s) \) given by QMC (Tanatar-Ceperley results for the fully spin-polarized 2DES for \( r_s \) up tp 30 were used in [15]). Once \( T_q \), which maps the \( T = 0 \) quantum fluid to a classical fluid is known, finite-\( T \) fluids are calculated from classical fluids at the temperature \( T_{eq} = (T^2 + T_q^2)^{1/2} \), as justified in ref. [14]. We have shown [13, 15] that the classical PDFs are in very close agreement with the quantum fluid PDFs obtained via QMC. The success of the method (refs. [13–16]) for 2-D and 3-D electrons, hydrogen fluids, and for 4-component 2-D electron fluids as judged by comparison with QMC data establishes it to be a well controlled, highly reliable method. The PDFs are easily used in a coupling-constant integration for the exchange-correlation free energies \( F_{xc} \). Our finite-\( T \) method accurately recovers the low-\( T \) logarithmic terms in \( F_c \) which cancel with corresponding terms in \( F_x \). This method, based on a classical mapping of the quantum calculation to an HNC calculation is called CHNC [1, 13–15].

Evaluation of \( m^* \) and \( g^* \). The evaluation of the susceptibility enhancement \( m^* g^* \) uses the \( T = 0 \) results for the exchange-correlation energy \( \epsilon_{xc}(r_s, \zeta) \). This is expressed in terms of \( \epsilon_{xc}(r_s, 0) \) and \( r_{xc}(r_s, 1) \), and a polarization factor \( P(r_s, \zeta) \) given in Eq. (6) of Ref. [15]. Using Hartree units, the ratio of the static spin susceptibility to the ideal (Pauli) spin susceptibility

\[
\frac{\chi_{spin}}{\chi_{spin, ideal}} = \frac{m^* g^*}{m^* g^*_{ideal}}.
\]
The effective mass and the $g$-factor

\[
\frac{K^0}{K} = (m^* g^*)^{-1} = 1 + r_s^2 \partial^2 \epsilon_{xc} / \partial \zeta^2.
\]

(2)

The specific heats are obtained as the second-T derivatives of the interacting and ideal Helmholtz $F(r_s, T)$. Here $T$ is the physical temperature and not $T_{cf}$. The latter is used only in the classical map to obtain the PDFs. $F_x(r_s, T)$ has a logarithmic term of the form $T^2 \log(T)$ which is cancelled by a similar term in $F_c(r_s, T)$. That is,

\[
F_x = A_x + B_xt^2 \log(t) - C_xt^2, \quad t = T/E_F
\]

(4)

\[
F_c = A_c + B_ct^2 \log(t) - C_xt^2, \quad B_c = -B_x.
\]

(5)

This cancellation holds to 85-95\% in our numerical CHNC results, for the range $r_s = 5 - 30$, $0 < t < 0.25$. Thus, at $r_s = 15$ and 25, $(B_x, B_c)$ are (-0.0258, 0.0228), and (-0.0155, 0.0142). If Hubbard-type finite-$T$ RPA were used in the self-energy, the cancellation is quite poor, even at low-$r_s$. These logarithmic terms and the $m^*$ have also been studied by Geldart et al., using CHNC [21]. Multi-valley systems- Shashkin et al. [7], also [23], have studied clean low-density 2-valley 2DES in Si-MOSFETs. The two valleys are assumed degenerate [24]. It is found [7] that the $m^*$ is strongly enhanced, while $g^*$ shows little change. The enhanced $m^*$ is independent of $\zeta$. These results, “contrary to normal expectations”, are reproduced by our coupled-mode theory of two valleys.
Two equivalent valleys and two spins imply 10 different PDFs, \( g_{ij}^{uv} \), where \( u, v \) are valley indices. Such a calculation for each \( r_s, \zeta, T \) and many values of the coupling constant is laborious. A simpler procedure using just three PDFs is possible. Even if \( \zeta \neq 0 \), each valley has a density \( n/2 \). Thus the 2-valley system may be made up from the known properties of the one-valley (two-spin) 2DESs coupled together by their Coulomb interaction. The individual 1-valley correlation free energies \( F_c^u, F_c^v \) are known from QMC and CHNC results. The inter-valley term for a system with a total density \( n \), and valley densities \( n/2 \) is not known. Here we present a simple approximation validated by calculating the 2-valley compressibility in the same way and comparing with the QMC data of Conti et al [8]. There is no exchange interaction between up-spin and down-spin electrons in the one-valley system, and the spin densities are \( n/2 \) at \( \zeta = 0 \). Hence, since \( F_c^u(n/2), F_c^v(n/2), \) and \( F_c(n, \zeta = 0, \{g_{12}\}) \) for the one-valley system are known, we build up the 2-valley system within the assumption that \( F_c(n, \zeta = 0) \) can be used for the inter-valley contribution to the \( F_c \) of the 4-component (i.e., 2-valley) system. In a full 4-component CHNC calculation, the inter-valley interaction is switched on via a coupling constant integration. This effect can be recovered within linear response by developing the coupled-mode 2-valley response functions. An analogous coupled-mode problem arises in electron-hole systems (see Vashishta et al [22]).

The total (spin or charge) density-fluctuation spectrum of the electrons in a given (single) valley \( v \) is described by the response functions \( \chi_v = \chi_v^0/D_v \), where \( \chi_v^0 \) is the 2-D Lindhard function weighted appropriately with the square of the Bohr magneton \( \mu_B \) or unity, and \( D_v \) is a corresponding denominator for each case. The Pauli susceptibility \( \chi_P \) is the long-wavelength limit \( \mu_B^2 \chi_v^0(k = 0) \). Let us consider a denominator of a response function (which may be the charge response \( \chi \), the proper polarization function \( \Pi \), or the spin susceptibility \( \chi_s \), depending on how the local-field factor \( G \) is specified). The denominator \( D_v = 1 - v_{\text{con}}(1 - G_v)\chi_v^0 \) and defines \( G_v \), the local-field factor (LFF, see [26]). We are only concerned with the static \( k \to 0 \) limit. Then \( G_v \) for \( \Pi \) are related to \( K^0/K \), while the \( G_v \) for \( \chi_s \) is given by \( \chi_P/\chi_s \), as in Eq. [2] and depends on the correlation free energy \( F_c \) of the one-valley 2DES. When two such 2DESs, described by \( \chi_v \) and \( \chi_u \) interact via the inter-valley term, coupled modes are formed. These modes are described by the zeros of a new denominator of the response function of the total 2-valley system. This coupled-mode form is [22]:

\[
\chi_{cm} = \frac{\chi_0 + \chi_v^0 + v_{\text{con}}^2 \chi_u \chi_v^0 (\Sigma G_{uv})}{D_{cm}} \quad (6)
\]

\[
\Sigma G_{uv} = G_a + G_v - G_{uv} - G_{vu} \quad (7)
\]

\[
D_{cm} = D_u D_v - v_{\text{con}}^2 \chi_u \chi_v (1 - G_{uv})(1 - G_{vu}) \quad (8)
\]

Here \( G_{uv} \) is an LFF arising from the inter-valley term \( F_{uv} \) already discussed, and modeled by \( F_{12}(n, \zeta = 0) \) at \( k = 0 \). Hence we express the susceptibility enhancement \( \chi_s/\chi_P \) as \( \chi_{cm}/\chi_P \), and this is evaluated from the \( G_a, G_v \) and \( G_{uv} \). Equation [2] determines \( G_a = G_v \), where the correlation part involves the second derivative \( (r_s^2 d^2 F_c^v/d\xi^2) \). Similarly the cross term \( G_{uv} \) involves \( r_s^2 d^2 F_{12}^v(n, \zeta = 0)/d\xi^2 \). The 4-component QMC results of Ref. [8] for \( F_s(r_s, \zeta = 0, T = 0) \) enable us to calculate the compressibility ratio \( K^0/K \) of the 2-valley system directly. The coupled-mode theory, applied to the proper polarization function \( \Pi \) gives another evaluation \( K^0/K \). The agreement between the two methods is shown in Fig. [1]. A similar comparison for \( \chi_P/\chi_s \) is not possible as the QMC results are available only at \( \zeta = 0 \). However, the agreement between the two estimates of \( K^0/K \) validates our coupled-mode evaluation of 2-valley properties from the 1-valley energies. Thus the 2-valley results are constructed from the 1-valley CHNC energies (which agree closely with QMC data) which include the usual bridge contributions [15].

Results – In Fig. [2] we show \( \chi_s/\chi_P = m^* g^* \) for a single-valley system, as a function of the
density \( n \), and as a function of \( r_s \) (see [3]) at \( T = 0 \) for \( \zeta = 0 \). Our results, the experimental data of Zhu et al. [6], and QMC data, extracted from Fig. 2 of ref. [2] are displayed. The high density regime [27] is in agreement with standard theories and is not displayed.

For the Zhu et al. data we use their fitted form \( m^* g^* = (2.73 + 3.9 n \zeta) n^{-0.4} \) where the density \( n \) is in units of \( 10^{10} \) cm\(^{-2} \). The strong agreement between CHNC and the Zhu data is perhaps fortuitous since the results are quite sensitivity to the \( d^2/d\zeta^2 \) calculation to the energy differences \( \Delta E = E_c(\zeta = 1) - E_c(\zeta = 0) \) and the form of the polarization factor \( P(r_s, \zeta) \). The CHNC is calibrated to the Tenatar-Ceperley QMC which differs somewhat from the Attaccalite data. We have also plotted two CHNC curves where (see Eq [3]) the term \( r_s^2 \partial^2 \epsilon_{xx}/\partial \zeta^2 \) has been modified by \( \pm 2\% \). Clearly, errors in converting to \( r_s \), modification of exchange-correlation gradients by well-width effects and the presence of impurities etc., can produce such a change. The bottom panel (Fig. 2) shows the comparison against \( r_s \).

Zhu et al. report a \( \zeta \) dependence, but now they consider that the finiteness of the 2-D layer and orbital effects cannot be ignored in analysing field-dependent data [28]. As pointed out via the \( \pm 2\% \) plots in Fig 2 the sensitivity of \( \chi_P/\chi_s \) to small errors in the xc-energy gradient is also important. (Discussion of these and other data for \( m^* \) and \( g^* \), of Zhu’s thesis [6] will await their publication).

In our results, \( \chi_s/\chi_P \) is less sensitive to \( \zeta \) at high density, and very sensitive to \( \zeta \) at low density, approaching the \textit{para–ferro} transition. In fact, the second derivative in Eq.2 diverges at \( \zeta = 1 \).

A very different experimental picture is found in Si-2DESs [7]. The CHNC results for the coupled 2-valley 2DES are shown in Fig. 3. The top panel compares the \( m^* g^* = \chi_{cm}/\chi_P \) obtained from experiment and the coupled-mode analysis (the LFFS used are for the spin-spin response). The inset shows the shift of the simple uncoupled-valley curve to higher densities when the valley coupling is introduced. The conversion between density and \( r_s \) is discussed in ref. [3].

The middle panel (fig. 3) shows the \( m^* \) calculated from the finite-\( T \) analysis, with the sharp rise occurring at \( r_s \sim 5.4 \), i.e., density \( n_{ev} = 1 \times 10^{11} \)/cm\(^2 \). The inset shows the lack of \( \zeta \) dependence in \( m^* \) for three densities. This is because the physics is dominated by singlet interactions, as in the ambi-spin phase reported earlier [1]. The lower panel of Fig. 3 shows the flat \( g^* \) of the coupled-valley fluid, while the inset shows the usual increase of \( g^* \) in the uncoupled system as the density is reduced.

\textit{Conclusion–} We have presented results for the effective mass \( m^* \), and the Landé \( g^* \) factor of 2-D electron fluids, using an analytic method. Our results suggest that exchange effects dominate as \( r_s \) increases in 1-valley 2D system, enhancing \( g^* \) when the one-valley spin-response diverges. Correlation effects outweigh exchange in 2-valley systems where \( m^* \) is strongly enhanced and only weakly dependent on \( \zeta \). The tendency to form singlets already noted in the single 2DES [25] becomes stronger in the 2-valley 2DES where a coupled-valley state is formed. Our theoretical results depend only on the \( \epsilon_{xx}(r_s, \zeta, T) \) used in calculating \( \zeta \) and \( T \) derivatives, and invoke no fit parameters specific to this problem. However, the inter-valley energy \( F_{iv} \) was approximated via the \( F_{12}(\zeta = 0) \) of the one-valley inter-spin energy. As already noted, \( \chi/\chi_0 \) is quite sensitive to the evaluation of \( d^2/d\zeta^2 \). However, the agreement of the present model with experiment may prove useful in understanding the experimental results.

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Fig. 2 – The spin-susceptibility enhancement $\chi_s/\chi_P = m^* g^*$ in the 2DES. Top panel: comparison of experiment [6], QMC [2], and CHNC. Curves marked $\pm 2\%$ are CHNC predictions if the exchange-correlation contribution $r_s^2 \partial^2 \varepsilon_{xc}/\partial \zeta^2$ is modified by $\pm 2\%$. Bottom panel: CHNC results for $m^* g^*$ for 3 spin-polarization $\zeta$, and the experimental $\zeta=0$ data, plotted against $r_s$.

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Fig. 3 – Comparison of experiment [7] and theory for the 2-valley 2DES in Si-MOSFETs. The top panel shows $m^* g^*$, while the inset shows the shift of theoretical $m^* g^*$ curve to higher densities due to mode coupling. The middle panel shows $m^*$ which rises steeply at the onset of the spin-singlet coupled-valley state at $n_{cv} = 1 \times 10^{11}/\text{cm}^2$. The inset shows the insensitivity of $m^*$ to the spin-polarization for three densities. The bottom panel compares the experimental $g^*$ with theory.