Spin- and valley-dependent analysis of the two-dimensional low-density electron system in Si MOSFETs

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The two-dimensional electron system (2DES) in Si metal-oxide field-effect transistors consists of two distinct electron fluids interacting with each other. We calculate the total energy as a function of the density \( n \) and the spin polarization \( \zeta \) in the strongly correlated low-density regime, using a classical mapping to a hypernetted-chain (CHNC) equation inclusive of bridge terms. The ten distribution functions arising from spin and valley indices are calculated to obtain the total free energy, the chemical potential, the compressibility, and the spin susceptibility. The \( T=0 \) results are compared with the two-valley quantum Monte Carlo (QMC) data of Conti and Senatore [Europhys. Lett. 36, 695 (1996)] (at \( T=0, \zeta=0 \)) and found to be in excellent agreement. Unlike in the one-valley 2DES, it is shown that the unpolarized phase is always the stable phase in the two-valley system, right up to Wigner crystallization at \( r_s \sim 40 \). Hence \( g^* \) is insensitive to the spin polarization and to the density. The compressibility and the spin-susceptibility enhancement calculated from the free energy validate a simple approach to the two-valley response based on coupled-mode formation. The local-density approximation of density-functional theory is shown to fail, especially near \( r_s = 1 \), even though the 2DES is uniform. The spin-susceptibility enhancement calculated from the coupled-valley response and directly from the two-valley energies is discussed. The three methods, QMC, CHNC, and coupled-mode theory, agree closely. Our results contain no ad hoc fit parameters and lead to general agreement with available experimental results.

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I. INTRODUCTION

The two-dimensional electron systems (2DES) in GaAs-like structures, as well as those found in Si metal-oxide field-effect transistors (MOSFETs) access a wide range of electron densities under controlled conditions, providing a wealth of experimental observations.\(^1\) The nature of the physics depends on the “coupling parameter” \( \Gamma = (\text{potential energy})/(\text{kinetic energy}) \). The \( \Gamma \) for the 2DES at the density \( n \) happens to be equal to the mean-disk radius \( r_s = (\pi n)^{-1/2} \) per electron, expressed in effective atomic units that depend on the bandstructure mass \( m_b \) and “background” dielectric constant \( \varepsilon_{\infty} \). Thus \( \Gamma = r_s \) is used as a small parameter in Fermi-liquid-like perturbation approaches to the 2DES. In this paper \( r_s \) is simply the electron-disk radius and the perturbation theory is not used. The 2DES in GaAs-like structures will be called a simple 2DES or one-valley 2DES to distinguish it from the two-valley system found in, e.g., Si MOSFETs. The inversion layer adjacent to an oxide layer grown on the Si (001) surface contains two equivalent valleys which host two equivalent electron fluids. Various aspects of such multi-valley systems were studied\(^2\) by Sham and Nakayama, Rasolt \textit{et al.}, and others, mainly in the high-density limit. The simple 2DES is also a two-component system (two spin species), while the two-valley system involves four components and ten pair-distribution functions (PDFs).

In a recent study of the effective mass \( m^* \) and the effective Landé-\( g \) factor of the 2DES, the Coulomb coupling between the electrons of the two valleys was shown to have a dramatic effect at low densities when the coupling becomes large.\(^3\) In effect, the elementary excitations of the two fluids in the two valleys interact to form coupled modes, giving rise to new effects. It was shown experimentally\(^4\) that \( m^*g^* \) rises rapidly with decreasing density in Si MOSFETs, and that this rise is due to a dramatic increase in \( m^* \), independent of the spin polarization, while \( g^* \) remains essentially constant. Calculations for the Si system which account for the intervalley Coulomb coupling quantitatively predict\(^5\) the sharp increase in \( m^*g^* \). It was also shown that \( g^* \) remained essentially constant, in strong contrast to the behavior found theoretically for the simple one-valley 2DES.\(^3\) The effective mass was also shown to be practically independent of the spin polarization,\(^5\) in excellent agreement with the data of of Shashkin \textit{et al.}\(^4\) for Si MOSFETs. The enhancement of \( m^*g^* \) in the one-valley 2DES of GaAs-like systems is found to be dependent on the spin polarization,\(^5\) in strong contrast to the Si MOSFET case. Our calculations\(^3\) show that the physics of the one-valley system is dominated by the presence of a transition to a fully polarized state, which makes \( g^* \) increase rapidly with \( r_s \) as the transition density is approached. The two-valley system shows no such transition to the spin-polarized state and is relatively insensitive to the spin polarization.

The perturbation theory becomes questionable for \( r_s > 1 \). Instead, we use a direct evaluation of the total free energy \( F(n, \zeta, T) \). The second derivative of the total free energy \( F(n, \zeta, T) \) with respect to the spin polarization \( \zeta \) gives a value for \( m^*g^* \) of the two-valley system. This requires the \( \zeta \)-dependent two-valley energy, which is not yet available from quantum Monte Carlo (QMC) simulations. However, we can evaluate \( F(n, \zeta, T) \) using CHNC, and also show that the hypernetted-chain (CHNC) results agree with QMC data (available at \( \zeta = 0 \) and \( T=0 \)). Another approach, which avoids the need for a full four-component calculation is to build up the two-valley...
susceptibility by noting that the one-valley energy \( E(n, \xi, T) \) is available at \( T=0 \) from QMC, and at any \( T \neq 0 \) from CHNC. The coupling of the excitations in the two valleys can be included in the coupled response function in a standard way. Then we find that the increase in \( CHNC \). The coupling of the excitations in the two valleys is available at \( CHNC \) method is given in Sec. II. In Sec. III we discuss the static small-\( q \) limit of the spin response function provides the needed \( x_{ij} / x_{0} \).

The objective of this paper is to (i) present \( F(n, \xi) \) data for the two-valley system by a four-component CHNC calculation involving the ten pair distributions that are needed in the two-valley system, and establish the close agreement of the CHNC results with the QMC calculations, and (ii) construct the coupled-mode response functions using the well-established one-valley data, and show that these results are also validated by QMC and full four-component CHNC results. We will not present detailed finite-\( T \) calculations (and hence \( m^{*} \) calculations, as detailed in Ref. 3) in this paper, as such calculations would make the paper too long and unwieldy. Also, finite-\( T \) data are not presently available from QMC simulations for comparison. A brief account of the CHNC method is given in Sec. II. In Sec. III we discuss the construction of the coupled-mode response functions which use only the one-valley exchange-correlation data to obtain the two-valley behavior. The compressibility predicted via the small-\( q \) limit of the so constructed coupled-mode response is found to agree very well with that from QMC or the full four-component CHNC calculations. This validates the coupled-mode model used in the calculation (Ref. 3) of the \( m^{*} \) enhancement in Si MOSFETs. The full two-valley energy calculations enable us to examine the usual one-valley local-density approximation (LDA) in Si MOSFETs and the corrections arising from coupled-mode effects. Finally, we discuss the spin-susceptibility enhancement obtained from these calculations, and the question of relating the electron-disk radius \( r_{e} \) used in these calculations to the experimental densities. Although the main thrust of this study is for two-valley systems, we give comparisons with one-valley results, and with suitable experiments.

II. FOUR-COMPONENT CHNC CALCULATIONS FOR THE TWO-VALLEY ELECTRON FLUID

We consider a 2DES in a Si MOSFET at a total density \( n \), with \( r_{e}^{2} = 1/\pi n \), while the density in each valley \( v = a \) or \( b \), is taken to be \( n_{v} = n/2 \). Hence the \( r_{e} \) parameter in each valley becomes \( r_{a}^{2} = r_{b}^{2} = \sqrt{2} \). Thus we do not consider density polarizations leading to \( n_{a} \neq n_{b} \). Also, the electrons in both valleys have the same spin polarization \( \xi \) and the same temperature \( T \). This is consistent with recent studies that show that the valley splitting is very slight.\(^{6}\) If the two spin species are denoted by \( i = 1, 2 \), we have a four-component 2DES with ten independent PDFs, viz., \( g_{ij,ab}(\mathbf{r}) \). We define \( k = 1, 2 \) for the two spins in valley \( a \), and \( k = 3, 4 \) for the two spins in valley \( b \), and write the PDFs as \( g_{k}(\mathbf{r}) \). The CHNC method for 2DES has been described fully in Ref. 7, where the quantum fluid at \( T=0 \) is considered to be equivalent to the classical fluid at a quantum temperature \( T_{q}(\mathbf{r}) \). It contains the essential “many-body” input to the problem. In a brief outline, in CHNC we assume that the 2D electrons are mapped onto a classical system where the distribution functions are given by a finite-\( T \) classical density functional form,

\[
g_{k}(\mathbf{r}) = e^{-\beta P(\mathbf{r})g_{k}(\mathbf{r}) + V_{\text{Coul}}(\mathbf{r}) + V_{c}(\mathbf{r})},
\]

Here, \( \beta P(\mathbf{r}) \) is a “Pauli exclusion potential,” which acts only for parallel spins, i.e., if \( k = l \). It is constructed such that \( g_{k}(\mathbf{r}) \) becomes identical with the noninteracting PDF, viz., \( g_{0}(\mathbf{r}) \), which is known from quantum mechanics when the Coulomb interaction \( V_{\text{Coul}}(\mathbf{r}) \) and the associated correlation corrections \( V_{c}(\mathbf{r}) \) are zero. The Coulomb interaction between two electrons in the equivalent classical picture involves a correction arising from their mutual diffraction effects. Thus \( V_{\text{Coul}}(\mathbf{r}) \) is obtained by solving a two-electron Schrodinger equation. The result is parametrized by the form,\(^{7}\)

\[
V_{\text{Coul}}(\mathbf{r}) = (1/\xi)(1 - \exp(-k_{B}T)),
\]

\[
k_{B} = 1.1587T_{c}^{1/2},
\]

\[
k_{B} = (2\pi m^{*}T_{c}^{1/2})^{1/2},
\]

\[
T_{c}^{1/2} = (T_{c}^{2} + T_{c}^{2}).
\]

Here \( k_{B} \) is the de Broglie momentum of the scattering pair with the effective pair mass \( m^{*} = 1/2 \), and \( T_{c} \) is the classical fluid temperature which reduces to \( T_{q} \) at \( T=0 \). The correlation potential \( V_{c}(\mathbf{r}) \) occurring in Eq. (1) is taken to be the sum of hypernetted-chain diagrams inclusive of a bridge term. Thus \( V_{c} \) is nonlocal and is a function of the \( g_{k}(\mathbf{r}) \), which have to be self-consistently calculated. The bridge term mimics the higher-order correlations which are not captured by the simplest HNC equations. These were shown to be important in 2D electron systems in Ref. 7. Particles having identical indices \( k = l \) are restricted from close approach by the Pauli exclusion effect modeled by \( P(\mathbf{r}) \delta(lk) \). However, singlet pairs of electrons, or electrons in two different valleys, contribute to strong Coulomb correlations, and hence a bridge term is included in all such “off-diagonal” PDFs. The bridge term \( B_{k}(\mathbf{r}) \) for \( k \neq l \) applies to six different PDFs, and we have taken this to be given by the usual hard-disk functional form discussed in Ref. 7. (Khanh and Totsuji\(^{8}\) have studied a more detailed implementation of the hard-disk bridge function in CHNC, while Bulutay and Tanatar\(^{9}\) have studied the 2D CHNC without a bridge correction.) It should be emphasized that both the HNC approximation, as well as the need for a bridge function, can be avoided by using the classical mapping to a quantum fluid (CMQF), where we use classical molecular dynamics (MD) to generate the PDFs of the classical fluid under consideration. In such a scheme we use the pair potential given by Eq. (2), plus the Pauli potential in an MD simulation for a classical plasma at the temperature \( T_{c} \). Such a CMQF-MD scheme would be numerically more demanding than the CHNC, much simpler than the full QMC simulations, and have the advantage of not making the HNC+bridge approximations. However, the two-valley (four-component) system examined here has been studied by QMC and we use those results to confirm the validity of our methods.
TABLE I. Comparison of the total energy $\epsilon_{\text{tot}}(r_s)$ and the correlation energy $\epsilon_c(r_s)$, in atomic units at $T=0, \zeta=0$ for the two-valley 2DES obtained from CHNC, with the QMC data of Conti et al. (Ref. 10).

<table>
<thead>
<tr>
<th>$r_s$</th>
<th>$\epsilon_{\text{tot}}(r_s)^{\text{QMC}}$</th>
<th>$\epsilon_{\text{tot}}(r_s)^{\text{CHNC}}$</th>
<th>$\epsilon_c(r_s)^{\text{QMC}}$</th>
<th>$\epsilon_c(r_s)^{\text{CHNC}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>−0.29302</td>
<td>−0.29172</td>
<td>−0.14315</td>
<td>−0.14202</td>
</tr>
<tr>
<td>10.0</td>
<td>−0.08611</td>
<td>−0.08647</td>
<td>−0.04607</td>
<td>−0.04649</td>
</tr>
<tr>
<td>20.0</td>
<td>−0.04641</td>
<td>−0.04643</td>
<td>−0.02577</td>
<td>−0.02581</td>
</tr>
<tr>
<td>30.0</td>
<td>−0.03196</td>
<td>−0.03183</td>
<td>−0.01806</td>
<td>−0.01795</td>
</tr>
</tbody>
</table>

The main difference in the physics of the one-valley system and the two-valley system arises from the preponderance of direct Coulomb interactions (from six PDFs in the two-valley, and one in the one-valley) over the exchange interactions (from four PDFs in the two-valley, and two in the one-valley). This is the main reason for the lack of a transition to a stable $\zeta=1$ state at low density. Since the transition to a $\zeta=1$ state does not occur as $r_s$ increases, the $g^*$ remains insensitive to increasing $r_s$, as found theoretically, and experimentally.

The ten coupled equations for $g_{\alpha}(r_z)$ are self-consistently solved for many values of the coupling constant $\lambda$ applied to the Coulomb interaction. Usually seven to 13 values are sufficient, depending on the convergence. The resulting $g_{\alpha}(r_z)$ are used in the adiabatic connection formula to determine the exchange-correlation free energy of the two-valley 2DES. While our calculations are easily carried out for any value of $\zeta, T,$ and $r_s$, the four-component QMC calculations at finite $T, \zeta$ are a major computational undertaking which has not been attempted. However, at $T=0, \zeta=0$, Conti and Senatore have presented QMC results for 2D electron bilayers separated by a distance $d_L$. They give total energies and also a fit to the correlation energy/electron $\epsilon_c(r_s, \zeta=0, T=0)$ at $d_L=0$, i.e. the case where both electron gases reside in the same layer. In Table I we compare the four-component CHNC with the available four-component QMC data at $d_L=0$. The energies $\epsilon_c(r_s)^{\text{QMC}}$ are from the Rapisarda-Senatore fit formula with the parameters quoted in Table I of Ref. 10.

The CHNC method provides a simple and accurate approach to the treatment of exchange and correlation in the four-component system. In situations where QMC results are available for the correlation energies, we adopt the CHNC parametrizations. Thus one may use the parametrization of $\epsilon_c$ given by Conti and Senatore for the $T=0, \zeta=0$ case. For $r_s > 1$ applications, the Tanatar-Ceperley form may also be used for parametrizing the two-valley system as well, with the parameter values $a_0=-0.40242, a_1=1.1319, a_2=1.3945$, and $a_3=0.67883$ fitted to a database from $r_s=1$ to 30.

The $T=0, \zeta=1$ case is particularly interesting, since this system (i.e., a two-valley system at density $n$) is mathematically identical to the one-valley system at the same density, but with $\zeta=0$, for the Hamiltonian considered by Conti and Senatore, and by us in this study. In this case the two-valley system has a twofold symmetry since the energy is the same, irrespective of the orientation of the spin in each valley. That is, $\zeta=1$ means all the spins in valley $a$ are oriented, while all the spins in valley $b$ are also oriented, but independently of the orientation of the spins in $a$. This degeneracy would be resolved in real Si MOSFETs, but not in the model used here, or in Conti and Senatore. For instance, the three-body correlations for intervalley interactions may be slightly different from those in the intravalley interactions, and hence may require two different bridge parameters, to be determined variationally by an energy minimization using the hard-disk reference fluid approach. We have not done this, and simply used the same bridge parameter as in Ref. 7 for all interactions. In the QMC calculation this would require independent optimization of the model for back-flow corrections. Finally, the correlation energy of the fully spin-polarized (degenerate) two-valley system can be parametrized using the Tanatar-Ceperley form with $a_0=-0.19162$, $a_1=3.6123$, $a_2=1.9936$, and $a_3=1.4714$ in atomic units.

### A. The energy of unpolarized and polarized phases

The $T=0$ correlation energy at finite values of $\zeta$ were calculated using the CHNC procedure and compared with the values predicted from the polarization factor used for the one-valley 2DES. This has the form

$$p(r_s, \zeta) = \frac{\epsilon_c(r_s, \zeta) - \epsilon_c(r_s, 0)}{\epsilon_c(r_s, 1) - \epsilon_c(r_s, 0)} = \frac{\zeta \epsilon_c(0) + \epsilon_c(r_s) - 2}{2 \epsilon_c(0) - 2},$$

$$\alpha(r_s) = C_1 - C_2/r_{z_1} + C_3/r_{z_1}^{2/3} - C_4/r_{z_1}^{13}. \quad (5)$$

Here, $\zeta=(1 \pm \zeta_0)$. It turns out that the coefficients $C_1-C_4$ obtained for the one-valley 2DES, i.e., 1.5404, 0.030544, 0.29621, and 0.23905, respectively, work quite well for the two-valley system well, even at high $r_s$. Thus, using the TC-type fit formula for the two-valley $\epsilon_c(r_s, \zeta=1)$ and $\epsilon_c(r_s, \zeta=0)$, the estimated values of $\epsilon_c(r_s, \zeta)$ and the CHNC values are given in Table II. Our spin-dependent function respects the Hartree-Fock limit. Attaccalite et al. have given a functional representation for 2D spin-polarized systems, where they have attempted to carefully respect the high-density and low-density behaviors of the xc energy. We find that their parametrization could also be adapted to the present problem.

The finite-$\zeta$ calculations show that there is no ferromagnetic phase transition in this system at $T=0$, since the total energy of the $\zeta=0$ phase is always more negative than any polarized phase. This is expected from the dominance of the
TABLE III. Comparison of the exchange-correlation energy $\epsilon_{xc}(r_s)$ per electron, and the Kohn-Sham potential $V_{xc}(r_s)$, in atomic units at $T=0$, $\zeta=0$ for the two-valley 2DES obtained from QMC fit or CHNC, and from the LDA.

<table>
<thead>
<tr>
<th>$r_s$</th>
<th>$\epsilon_{xc}(r_s)^{\text{LDA}}$</th>
<th>$\epsilon_{xc}(r_s)^{\text{QMC}}$</th>
<th>$V_{xc}(r_s)^{\text{LDA}}$</th>
<th>$V_{xc}(r_s)^{\text{QMC}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>$-0.70960$</td>
<td>$-0.62843$</td>
<td>$-1.02897$</td>
<td>$-0.88608$</td>
</tr>
<tr>
<td>2.0</td>
<td>$-0.38213$</td>
<td>$-0.35535$</td>
<td>$-0.55189$</td>
<td>$-0.50271$</td>
</tr>
<tr>
<td>10.0</td>
<td>$-0.09007$</td>
<td>$-0.08851$</td>
<td>$-0.13133$</td>
<td>$-0.12835$</td>
</tr>
<tr>
<td>20.0</td>
<td>$-0.04742$</td>
<td>$-0.04699$</td>
<td>$-0.06957$</td>
<td>$-0.06874$</td>
</tr>
</tbody>
</table>

many off-diagonal terms contributing to direct Coulomb interactions, but without exchange interactions. This was pointed out in Ref. 3, where the insensitivity of $m^*g^*$ to $\zeta$ obtained from the theory was in excellent agreement with the experiments of Shashkin et al.4 The stabilization energy $\Delta E$ of the $\zeta=0$ phase with respect to the fully polarized phase is $0.12734 \times 10^3$ a.u. at $r_s=25$, and diminishes to $0.89929 \times 10^3$ a.u. at $r_s=40$. These are very small energy differences and within the error of the CHNC method, and possibly of the two-valley QMC calculations. However, the pattern of stability of the $\zeta=0$ phase holds for all $r_s$ investigated. We arrive at the conclusion: there is no spin-phase transition in the two-valley system.13

B. LDA-type calculations for Si MOSFETs

In most density-functional calculations of Si/SiO$_2$ quantum wells, the Kohn-Sham exchange-correlation (xc) potential $V_{xc}(r)$ is calculated using the LDA, where the total density $n(r)$ is considered without taking account of the valley degeneracy. In effect, the electron gas is assumed to be a single electron gas at a density $r_s$, and its exchange-correlation energy $\epsilon_{xc}(r_s)$ and the Kohn-Sham potential $V_{xc}(r_s)$ are calculated at the given density. [We recall that $V_{xc}(r)$ is simply the xc contribution to the chemical potential $\mu_{xc}$.] Results for $\epsilon_{xc}$ and $\mu_{xc}$ for electrons in a Si MOSFET calculated correctly, i.e., taking account its degenerate valley structure, and in the usual LDA approach, are compared in Table III. The full chemical potential $\mu$, as well as the compressibility ratio $K^0/K$ calculated for the two-valley system, and that obtained within the LDA approach, are also shown in Fig. 1. It is noteworthy that the total chemical potential has a minimum near $r_{sm} \sim 1$. In effect, a low-density electron fluid ($r_s > r_{sm}$) whose chemical potential is equal to that of a high-density gas ($r_s < r_{sm}$) exists and this could lead to spontaneous density inhomogeneities in these systems.

When the actual electron densities in Si MOSFETs are converted to effective $r_s$ units (see below), the $r_s$ range 1–6 is the most important for device applications, and hence, overestimates in $V_{xc}$ contained in the usual LDA approach could be significant. This becomes even more significant in spin-density functional applications to Si-based nanostructures.

C. Pair-distribution functions in the Si-MOSFET system

The PDFs, denoted by $g_{kl}(r)$, embody the detailed particle correlations in the system. In Fig. 2 we display an illustrative set of pair-distribution functions. QMC-based PDFs have not been reported in the literature and hence we do not have a direct comparison. However, good agreement between CHNC and QMC-based PDFs have been found in other systems (e.g., 2DES, 3DES, and fluid hydrogen).7,14–16 For $\zeta=0$ the four diagonal PDFs $g_{kk}$ are identical, and similarly, all of the six off-diagonal PDFs are also identical. Hence there are actually only two distinct PDFs, just as in the single-valley case, where $g_{11}$ and $g_{12}$ define the $\zeta=0$ case. These are shown for $r_s=2, 10$, and 20 in the top panel of Fig. 2. It is also clear that the correlation effects are mainly determined by the off-diagonal PDFs. This is in keeping with our understanding that singlet-like correlations are more important than parallel spin (ferromagnetic) correlations in the two-valley system. At finite $\zeta$ there are five independent PDFs. There are two independent diagonal PDFs, $g_{11}=g_{13}$ and $g_{22}=g_{44}$. The three independent off-diagonals are $g_{12}=g_{23}=g_{34}=g_{14}=g_{13}$, and $g_{24}$. These are shown for the case $r_s=10$ and $\zeta=0.5$ in the lower panel of Fig. 2.

III. RESPONSE FUNCTIONS

In the following we discuss the linear response functions, since the static small-$k$ limit can be related to the derivatives of the total energies that were calculated from CHNC or QMC, if available. This enables us to verify a simple procedure for the construction of the two-valley response functions using only single-valley exchange correlation data.5

FIG. 1. Left panels: Comparison of the total chemical potential $\mu$, i.e., the total Kohn-Sham potential, calculated at the total density $n$ and $r_s$, for the two-valley system, and if the LDA were used (labeled 1-valley), ignoring the two-valley nature. Right panels: Same for the compressibility ratio.
The density-density response function \( \chi(k, \omega) \) will be called the \( d-d \) response for brevity. We emphasize that this is not a “fluctuation” analysis, but a strictly thermodynamic approach based on the small-\( k \) limit of the static response functions, as discussed below.

The response function is expressed in terms of a reference “zero-order” \( \chi^{0}_R(k, \omega) \) and a local-field factor (LFF), denoted by \( G(k, \omega) \).

\[
\chi(k, \omega) = \chi^{0}_R(k, \omega)/[1 - V_k(1 - G_d(k, \omega))\chi^{0}_R(k, \omega)].
\]

(6)

The \( s-s \) response (or “spin susceptibility”) is written as

\[
\chi_s(k, \omega) = -\mu_B^2\chi^{0}_R(k, \omega)/[1 - V_k(1 - G_s(k, \omega))\chi^{0}_R(k, \omega)],
\]

(7)

where \( \mu_B \) is the Bohr magneton. Note that our definition of the spin LFF differs somewhat from a commonly used definition.\(^{17}\) Our form makes the \( d-d \) and \( s-s \) LFFs appear formally similar, at least at this stage. Hence, a single discussion applies to both, and we drop the subscripts \( d \) and \( s \). The reference function \( \chi^{0}_R(k, \omega) \) has the form

\[
\chi^{0}_R(k, \omega) = \sum_{\vec{k},\sigma} \frac{n_{\sigma,\vec{k}} - n_{\sigma,\vec{k}+\vec{q}}}{\omega + \epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}}.
\]

(8)

Here \( \vec{k}, \vec{q} \) are two-dimensional vectors, while the corresponding single-particle energies are denoted by \( \epsilon_{\vec{k}} \), etc. The Fermi occupation number \( n_{\sigma,\vec{k}} \) may be chosen to be the noninteracting value, in which case \( \chi^{0}_R \) is the 2D Lindhard function.\(^{2}\) An alternative is to use the fully interacting density, evaluated from the fully interacting chemical potential, as in the density-functional theory (DFT).

The small-\( k \) limits of the local-field factors \( G_d(k, \omega) \) and \( G_s(k, \omega) \) can be obtained from the second derivatives of the exchange-correlation free-energy functional \( F_{xc}(n, \zeta) \) of DFT, with respect to the charge densities or the spin densities.\(^{18}\) These second-order derivatives, together with the second derivative of \( F_{xc}(n, \zeta) \) with respect to \( T \) for a two-valley system, were used in our \( m^* \) and \( g^* \) calculations reported in Ref. 3, using the CHNC technique. Here we look at the compressibility and spin susceptibility of the two-valley system obtained from the small-\( k \) limit of the coupled-mode response function (built up from one-valley data) and compare it with that obtained directly from the two-valley CHNC and QMC.

A. Response functions of the two-valley system

The theory of the one-valley fluid can be used for the two-valley (four-component) fluid if there is no valley polarization (i.e., the two valleys are assumed equivalent although distinct), as in Ref. 3. As this may not be completely clear from the abbreviated discussion in Ref. 3, we present some details here.

In the theory of classical fluids, the response functions are simply related to the structure factors, while the LFFs are simply related to the direct correlation functions of Ornstein-Zernike (OZ) theory. Since this paper is directed more towards electron-fluid studies, we follow the language of the LFFs and the related response methodology, rather than the OZ presentation.

Let us indicate the species (which may be a valley index or a spin index) by \( u \) or \( v \), taking the values 1 and 2, and consider a weak external potential \( \phi_u(\vec{k}, \omega) \) that acts only on the electrons of species \( v \). The external potential induces density deviations \( \delta n_u(\vec{k}, \omega) \) such that:\(^{19}\)

\[
\delta n_u(\vec{k}, \omega) = \sum_v X_{uv}(\vec{k}, \omega)i\phi_u(\vec{k}, \omega).
\]

(9)

These equations define the linear \( d-d \) response functions involving the species \( u \) and \( v \). The longitudinal dielectric function \( e(\vec{k}, \omega) \) is now given by

\[
1/e(\vec{k}, \omega) = 1 + V_k \sum_{u,v} X_{uv}(\vec{k}, \omega).
\]

(10)

Here \( V_k \) is the 2D Coulomb interaction \( 2\pi/k \). Note that we are using effective atomic units (Hartrees, etc.), such that \( e^2 \) divided by the background dielectric constant is taken to be unity (see Sec. IV). To relate the response functions to the
local fields, we consider the effective potentials $U_{\nu}(\vec{k}, \omega)$ such that

$$U_{\nu}(\vec{k}, \omega) = V_{\nu}\left[1 - G_{\nu\nu}(\vec{k}, \omega)\right] \delta n_{\nu}(\vec{k}, \omega).$$  \hspace{1cm} (11)

Thus the bare Coulomb interaction between the particles of type $\nu$ and $\nu$ is modified by the LFFs $G_{\nu\nu}$. Hence, we can write the density deviations $\delta n_{\nu}(\vec{k}, \omega)$ in terms of the effective potentials and the zeroth-order response functions as follows (we drop the $\vec{k}, \omega$ labels for brevity):

$$\delta n_{\nu} = \chi_{\alpha}^{0} \left[ \phi_{\alpha} + V_{\nu} \sum_{\nu} (1 - G_{\nu\nu}) \delta n_{\nu} \right].$$  \hspace{1cm} (12)

Now, by a comparison of the Eqs. (9) and (12), we can write down the response functions of the coupled two-component system in terms of the zeroth-order response functions and the LFFs.

$$\chi_{11} = \chi_{1}^{0} d_{1}/D, \quad \chi_{22} = \chi_{2}^{0} d_{1}/D, \quad \chi_{12} = V_{\nu} \chi_{12}^{0}[1 - G_{12}]/D, \quad d_{1} = 1 - V_{\nu} \chi_{11}^{0}[1 - G_{1}], \quad d_{12} = V_{\nu} \chi_{12}^{0}[1 - G_{12}], \quad D = d_{1}d_{2} - d_{12}d_{21}.$$  \hspace{1cm} (13-17)

We have suppressed the $\vec{k}, \omega$ dependence in the above equations, and also not explicitly given $\chi_{11}$, $d_{2}$, and $d_{21}$ for brevity. We now define a total coupled-mode response function $\chi_{T}(\vec{k}, \omega)$ via

$$1/e(\vec{k}, \omega) = 1 + V_{\nu} \chi_{T}(\vec{k}, \omega).$$  \hspace{1cm} (18)

Then the total two-component 2DES response is given by

$$\chi_{T} = \left[ \chi_{1}^{0} + \chi_{2}^{0} + V_{\nu} \chi_{12}^{0} G_{2} \right]/D,$$  \hspace{1cm} (19)

$$G_{2} = G_{11} + G_{22} - G_{12} - G_{21}.$$  \hspace{1cm} (20)

The evaluation of $\chi_{T}$ using only one-valley xc-data is our objective. In the following, we sometimes denote $\chi_{T}$ by $\chi_{cm}$ to emphasize the coupled-mode nature of the total response. If we are dealing with a simple (one-valley) electron fluid, e.g., a partially spin-polarized electron gas, the species index $\nu$ is simply the spin index. Notice that the coupling between the two systems (be they spins or valleys) replaces the individual denominators $d_{1}$ and $d_{2}$ by a new denominator $D$, common to both systems, and containing the cross terms $d_{ij}$. That is, instead of the two sets of excitations given by the zeros of $d_{1}$ and $d_{2}$, we now have a common set of “coupled-mode” excitations defined by the zeros of $D$. We emphasize that in this analysis we have not used any form of CHNC theory.

All the response functions prior to the switching on of the Coulomb interaction between the two valleys are known. The problem is to determine the cross terms $d_{ij}$, i.e., the intervalley term, $d_{iv}$, occurring in the coupled-mode denominator $D$, using only the free-energy data for a single valley. If we consider the small-$k$ limit, we see that the terms $d_{ij}$ occurring in $D$ are directly related to the second-density derivative or magnetization derivative of the free-energy contributions $F_{ij}$ arising from the PDFs $g_{ij}$. We know these individual free-energy contributions for the one-valley problem.

Let us first consider the small-$k$ limit of the static response functions to make contact with the compressibility and susceptibility sum rules.

B. Small-k limit of the static response

The small-$k$ behavior of the static response is related to the second derivative with respect to the density (or magnetization), and this provides well-known sum rules that we exploit here. For simplicity, and for comparison with the degenerate two-valley case, let us review the one-valley paramagnetic case $\xi=0$, and consider the calculation of the small-$k$, static ($\omega=0$) limit of the simple (one-valley) response function,

$$\chi_{\nu}(n_{\nu}) = \chi_{\nu}^{0}(n_{\nu})[1 - V_{\nu}(1 - G_{\nu\nu})\chi_{\nu}^{0}(n_{\nu})].$$  \hspace{1cm} (21)

The density-density response function is associated with the proper polarization function $\Pi_{\nu}$. Dropping the species subscript $\nu$ for the present, we have

$$\Pi = \Pi_{0}^{0}/(1 + V_{\nu} G_{\Pi_{0}}^{0}),$$  \hspace{1cm} (22)

$$\Pi_{0}^{0} = -\chi^{0}. $$  \hspace{1cm} (23)

The small-$k$ behavior of this function states that

$$\Pi / \Pi_{0} = \kappa / \kappa_{0}. $$  \hspace{1cm} (24)

The compressibility $\kappa$ is calculated via the chemical potential $\mu$, starting from the total free energy per unit volume obtained from the CHNC calculation.

$$F = F_{0} + F_{x} + F_{c}, $$  \hspace{1cm} (25)

$$F = \sum_{\nu} n_{\nu} [\epsilon_{\nu}^{0}(n_{\nu}) + \epsilon_{\nu}^{c}(n_{\nu})] + n \epsilon_{s}(n), $$  \hspace{1cm} (26)

$$\epsilon_{\nu}^{c} = (1 + \zeta^{2})/2\nu^{2}, $$  \hspace{1cm} (27)

$$\epsilon_{s} = -\frac{2\sqrt{2}}{3\pi n_{s}} \left[ (1 + \zeta)^{3/2} + (1 - \zeta)^{3/2} \right], $$  \hspace{1cm} (28)

$$\mu = \frac{dF}{dn} = \mu_{0} + \mu_{x} + \mu_{c}. $$  \hspace{1cm} (29)

$$1/\kappa = n^{2} \frac{d\mu}{dn}. $$  \hspace{1cm} (30)

At $T=0$, the chemical potential is given (in Hartrees) by

$$\mu = n_{s} \pi - 2(2/\pi)^{1/2} n_{v}^{1/2} + \mu_{c}. $$  \hspace{1cm} (31)

The compressibility calculated directly from the four-component calculation should agree with that obtained from the coupled-valley formalism. There, the small-$k$ limit of the
denominator of the density-density proper-polarization function is given by

\[ 1 + V_d G_d^0 = \kappa / \kappa_0. \]

Here \( G_d \) is the LFF of the density-density polarization function. Hence the denominator \( d_1 \) or \( d_2 \) of the \( d-d \) response occurring in Eq. (13), for any particular species is available for the density-density response function in each valley. But the cross density-density LFFs, e.g., \( G_{12} \), and the cross-denominators \( d_{12} \) needed to form the coupled-valley forms are not yet specified.

In the case of the spin susceptibility \( \chi_s \), the role played by the compressibility is taken over by the spin stiffness, which is the second derivative of the free energy \( F \) with respect to the spin polarization \( \xi \). Here we have, for a single valley,

\[ \chi_s / \chi_p = 1 + d^2 \left( \epsilon_p^2 F_{xc} \right) d\xi^2. \]  \hspace{1cm} (32)

Hence the denominators \( d_1 \) and \( d_2 \) of the spin susceptibilities of both 2DES are known, at the valley densities \( n_u = n_v = n/2 \), from a simple CHNC calculation or from a QMC energy parametrization. However, here again the cross terms \( d_{12} \) and \( d_{21} \) (which are equal) needed to complete the calculation of the coupled susceptibility [Eqs. (13) and (19)] are not yet specified.

The cross term for the \( d-d \) response, or for the \( s-s \) response, can be calculated if the free-energy contribution \( F_{xc} \) arising from the Coulomb interaction among the electrons in the two valleys is known. The interaction is among the electrons of valley \( u \), at density \( n/2 \), and the electrons of valley \( v \) at density \( n/2 \). The intervalley free-energy contribution \( F_{uv}(n/2,n/2) \) is purely Coulombic, and hence, it is clearly analogous to the correlation free-energy term arising from the antiparallel-spin PDF, i.e., \( g_{12}(n,\xi = 0) \) of the simple one-valley 2DES at density \( n \) with two spin species. The case \( \xi = 0 \) ensures that the total density is split as \( n_u = n_v = n/2 \). Thus the \( d_{12} \) term needed for the spin-susceptibility calculation and the density-density response calculation are

\[ s-s d_{12} = d^2 \left( \epsilon_p^2 F_{xc}^{(12)} \right) d\xi^2, \] \hspace{1cm} (33)

\[ d-d d_{12} = -(2/\pi) d^2 F_{xc}^{(12)} / dn^2. \] \hspace{1cm} (34)

Note that \( d_1 \) is calculated from \( F_{xc}(n/2,\xi = 0) \), while \( d_{12} \) is from \( F_{xc}(n,\xi = 0) \) of the simple one-valley 2DES. Hence, knowing \( d_1, d_{12} \) (which are equal to \( d_2 \) and \( d_{21} \), since the valleys are degenerate), we can calculate the susceptibility enhancement \( \chi_s / \chi_p \), as well as the compressibility ratio \( \kappa / \kappa_0 \) of the interacting two-valley 2DES, without actually solving the coupled system of ten distribution functions needed in the full CHNC calculation of the four-component system.

1. Results for the compressibility ratio and the susceptibility ratio

We consider the compressibility ratio \( K_0 / K \) obtained by the coupled-mode analysis and from the two-valley QMC data,\(^{10}\) or equivalently, from the four-component CHNC data, in Fig. 3. The excellent agreement shows that the coupled-mode procedure for using the one-valley data to generate two-valley data is successful.

\[ \epsilon_p(r_s,\xi) = \epsilon_p(r_s,0) + [\epsilon_p(r_s,1) - \epsilon_p(r_s,0)] p(r_s,\xi), \]

\[ \frac{d^2 \epsilon_p(r_s,\xi)}{d\xi^2} = \Delta E(1,0) \frac{d^2 p(r_s,\xi)}{d\xi^2}. \]

Thus the energy difference between the polarized and unpolarized phases appears directly. This becomes zero in systems
like the one-valley 2DES that show a spin transition. Even in the two-valley system, where there is no transition to a stable \( z = 1 \) state, we can expect the calculated \( \frac{x_s}{x_P} \) or \( \frac{x_{cm}}{x_P} \) to be quite sensitive to \( D_{\epsilon 1,0} \), and to the details of the form of the \( z \)-dependent function. We find that this is very much the case. In Fig. 4 we display the coupled-mode evaluation of \( m^* g^* = x_{cm}/x_P \), with the value of \( x_s/x_P \) obtained from the \( z \)-second derivative of the correlation energy obtained from the full four-component calculation. We give curves labeled “four-component” (a), and (b), where the contribution from the \( d^2 \epsilon_c/dr^2 \)-derivative term differs by \( \sim 5\% \). Clearly, this small change has a drastic effect on the \( m^* g^* \) evaluation. We have also included the experimental results of Sashkin et al. for \( m^* g^* \) to show that the coupled-mode result, which differs slightly (see Fig. 3) from the full four-component result, is actually in close agreement with the experiment. In the lower panel of Fig. 3 we compare the two-valley correlation energy \( \epsilon_c(r_s, z=0) \) from the coupled-mode analysis and from the direct four-component QMC calculation. As expected, a small difference appears at low densities. This type of error is quite within the errors that are possible in the four-component

\[
\text{FIG. 4. Comparison of the susceptibility enhancement } \frac{x_{cm}}{x_P} = m^* g^* \text{ obtained from the coupled-mode approach and from the second } z \text{ derivative of the total free energy of the 4-component system. The curves marked “4-components” (a), (b) differ by } \sim 5\% \text{ in the value of the second } z \text{ derivative of the correlation energy, showing the strong sensitivity to this energy derivative.}
\]

QMC or the four-component CHNC, and in fitting to the polarization dependence of the numerically calculated correlation energies. We find that the coupled-mode approach, which involves a particular set of numerical (and model) approximations, happens to give the best agreement with Sashkin’s experiments, while the four-component CHNC calculation has a different set of numerical approximations and captures the coupled-mode formation via the OZ equations. These results imply that the simple ideal two-valley 2DES quite closely models the experimental Si-MOSFET samples, even though any actual differences in the two valleys, the effect of impurities, etc., are not included in the theory.

Coupled-mode formation implies that the excitation spectrum of the system no longer shows the features of the individual valleys, and hence is consistent with the conclusions of Ref. 6, where no evidence for intervalley scattering was seen. In this context, it is interesting to compare the spin-susceptibility enhancement if the two-valley nature of the 2DES is ignored and treated as if it were a one-valley system. Here, \( \zeta \) is the spin polarization. The experimental data of Zhu et al. for the one-valley GaAs 2DES are also shown.

\[
\text{FIG. 5. Comparison of the susceptibility enhancement } \frac{x_{cm}}{x_P} = m^* g^* \text{ if a given total electron density is assumed to be entirely in a one-valley 2DES, or equally divided to form a two-valley 2DES. Here, } \zeta \text{ is the spin polarization. The experimental data of Zhu et al. for the one-valley GaAs 2DES are also shown.}
\]
with the Attaccalite data, as well as the CHNC theory, for the range $3 < r_s < 10$. We also note that the CHNC method is based on the use of a quantum temperature $T_q$ fitted to the polarized 2D energies of Tanatar and Ceperley, rather than to the recent Attaccalite data. All this suggests that impurity and layer thickness effects, as well as the theoretical uncertainty in $\Delta (m^*g^*)$, lead to a “fan of uncertainty” of about 2%–3% in the estimate of $m^*g^*$. The width of the “fan” increases with $r_s$. We also remark that $\Delta (m^*g^*)$ is divergent for $\zeta = 1$. That is, the ease of polarizing the spins (the susceptibility) increases with the degree of polarization and becomes infinite at $\zeta = 1$. Hence, experimental results for higher values of $\zeta$ would be even more sensitive to various quenching effects which are not included in the idealized theory.

**IV. RELATION BETWEEN DENSITY $n$ AND THE $r_s$ PARAMETER IN Si MOSFETs**

In the 2DES of GaAs/AlAs-type structures, the dielectric constants of the two materials are nearly identical. The lattice constants are also well matched and hence the calculation of the effective atomic units needed in converting the experimental density $n$ to the effective electron-disk radius ($r_s$) can be carried out in an unambiguous, transparent way. This is important, since the many-body theory is formulated within the language of $r_s$ and effective atomic units. Of course, if the electron gas is not ideally thin, the 2DES becomes a 3D slab and further corrections are necessary.

Unlike in GaAs, the situation for Si MOSFETs is more complicated. The lattice mismatch between crystalline Si and most crystalline varieties (e.g., crystobalite) of SiO$_2$ turns out to be 35%–40%. The dielectric constants are also strongly mismatched, being $\sim 11.5$ and $\sim 3.9$ for Si and SiO$_2$. The large lattice mismatch ensures that there is no sharp Si/SiO$_2$ interface. The reconstruction of the Si atomic layers between the crystalline Si and the SiO$_2$ bulklike region still contains tetrahedral-bonding networks, but with strongly modified bond angles, bond lengths, etc., characteristic of the amorphization of the Si layers immediately adjacent to the oxide layer. Many decades of experimental and theoretical work have gone into sharpening our understanding of this interface. More recently, first-principles density-functional calculations by Carrier et al.\textsuperscript{23} starting from tight-binding models,\textsuperscript{24} have presented a clearer picture of the atomic arrangements near the interface region. A series of similar studies by Pasquerello et al.\textsuperscript{25} establish the geometry of the Si/SiO$_2$/vacuum interface. Thus, a reliable atomic model of the Si/SiO$_2$ interface obtained via geometry optimization of the total energy is now available.\textsuperscript{23} The essential point is that the Si/SiO$_2$ interface contains approximately five regions containing crystalline Si (c-Si), amorphized Si (a-Si), suboxide layers, amorphized silicon dioxide (a-SiO$_2$), and crystalline SiO$_2$. These are indicated schematically as,

$$[001]|z \rightarrow |c-Si|a-Si|suboxides|a-SiO$_2$(c-SiO$_2$].$$  \text{ (36)}

The amorphous (or bond distorted) regions of a-Si should be considered as the true insulator that separates the 2DES that reside at the interface between c-Si and a-Si. Let the location of this amorphization edge be at $z = z_a$. This edge can be
defined to within a few atomic planes within the first-principles theoretical models (see Ref. 23 for more details). If we are dealing with a thick electron gas, then envelope-function methods for describing the form factor may be reasonable. Otherwise, a more detailed atomic description involving Bloch functions is needed. In any case, if the electron gas is very thin, its growth-direction density profile may be considered to be \( \delta(z) \). That is, crystalline Si and \( a\)-Si flank the two sides of the 2D electron layer, with \( a\)-Si playing the role of the insulator. The valence bonds of the \( a\)-Si still form a quasirandom tetrahedral network, even though distorted, and hence the “background” dielectric constant of \( a\)-Si, is essentially that of Si. That is, the effective dielectric constant,

\[
\varepsilon = 0.5(\varepsilon_s + \varepsilon_m),
\]

(37)
only used for the 2DES in the MOSFET positioned at an abrupt Si/SiO\(_2\) interface, ignores the effect of the strong lattice mismatch of \( \sim 35\% - 40\% \). The second formula of Ando et al. (see Appendix of Ref. 2) for the conversion \( n \) to \( r_s \), using a mean \( \varepsilon \) of 7.7, is not recommended. Instead, the first formula of Ref. 2, i.e.,

\[
r_s a^* = 1.751 \left[ \frac{(10^{12} \text{ cm}^{-2})}{n_s} \right]^{1/2} \left[ \frac{11.5}{\varepsilon_{sc}} \right] \left[ \frac{m}{0.19m_0} \right],
\]

(38)
is clearly the one consistent with the first-principles atomic structure of the Si/SiO\(_2\) interface referred to above.\(^{23}\) If we look at the Si-MOSFET literature, we find that the formula which uses the average dielectric constant of 7.7, valid for the abrupt Si/SiO\(_2\) interface, has been used by a number of authors. These authors use a value of \( r_s \) increased by a factor of \( \sim 1.49 \) compared to what we recommend. Thus, Pudalov et al.\(^{26}\) and Okamoto et al.\(^{27}\) have used the mean dielectric constant of 7.7 for their calculation of \( r_s \). However, both these studies use the \( r_s \) parameter mainly as a plotting variable in the figures, and not for any many-body calculations. Hence a choice of \( r_s \), which differs from that used in our work by a factor of \( \sim 1.49 \), is immaterial. In the review article by Kravchenko and Sarachik,\(^{1}\) values of \( r_s \) are further modified by the experimentally obtained \( m^* \) to discuss the interactions in Si MOSFETs. Thus their \( r_s \) is explicitly modified to serve a specific purpose. Das Sarma and Hawang\(^{28}\) have also examined Si-MOSFET resistivities, using an impurity-scattering calculation which requires defining the effective background dielectric constant. They point out that their results are qualitative. Their results would not be affected by the choice of either formula given by Ref. 2, i.e., using \( \varepsilon = 7.7 \) or 11.5. Altschuler and Maslov\(^{29}\) actually consider the implications of the suboxide layer and how this could play a significant role in the theory. However, they too point out that their effort is essentially to indicate a “mechanism” rather than a theory of the metal-insulator physics of Si MOSFETs. Hence, once again, the results are too qualitative to make any difference. Similarly, the results of other workers\(^{30}\) also do not discriminate sufficiently to make the choice of \( \varepsilon \) a significant issue.

Another class of problems where the choice of the average dielectric constant is an issue is in calculating electric subband energies.\(^2\) Although the eigenvalues of the Kohn-Sham equation are not to be considered as effective excitation energies, such an assumption is often made. The input dielectric constant (which decides the effective \( r_s \)) enters into the exchange-correlation functions as well as the Poisson potential used. Most calculations are in the high-density regime, and it turns out that, given the uncertainties of the quantum-well potentials and other parameters, the results can be equally well explained by a range of values of the effective dielectric constant.

This situation becomes quite different when it comes to quantitative calculations for low-density MOSFETs, e.g., in the regime \( n = 1 \times 10^{11} \text{ electrons/cm}^2 \). Our CHNC calculations for \( m^* \) and \( g^* \) presented in Ref. 3 and Fig. 4 clearly favor the first formula, Eq. 38 of Ando et al.,\(^2\) as the correct formula. This is also the formula that is consistent with the Car-Parrinello optimized atomic structure of the Si/SiO\(_2\) interface obtained from the calculations of Carrier et al.\(^{23}\) and also of Pasquerello et al.\(^{25}\) We believe that the problem of the correct dielectric constant at the Si/SiO\(_2\) interface has received little scrutiny within the 2D electron community in the past, because there was no analytic many-body theory capable of giving quantitative results for low-density electron systems. Also, it is interesting to note that if the second formula of Ando et al. were used instead of the first formula that we recommend, then the calculated total \( r_s \) is close to the \( n/2 \) value (per valley, \( \sim 1.414 r_s \)) of \( r_s \) calculated by the first formula. This is consistent with the calculations that we advocate, at the Hartree-Fock level (i.e., at the single-electron level). This fact can also lead to some confusion in assessing the validity of numerical calculations.

The CHNC programs for electron-gas calculations mentioned here and in Ref. 7 may be accessed via the internet at the address given in Ref. 31.

V. CONCLUSIONS

We draw the following conclusions from this study. The CHNC method applied to a four-component electron fluid gives results in very close agreement with available diffusion Monte Carlo calculations, without the use of any adjustable parameters specific to the two-valley problem. The ground state of the two-valley 2DES is the unpolarized phase for all \( r_s \), and hence, there is no spin-polarization transition, in contrast to the one-valley 2DES. The coupled-mode approach to constructing the two-valley properties from one-valley data is also fully confirmed. The calculation of the spin-susceptibility enhancement \( \chi_s / \chi_P \) from the second \( \zeta \) derivative of the spin-dependent energy is found to be very sensitive to the energy difference between the polarized and unpolarized phases and to the form of the polarization dependence. Errors in the assignment of the \( r_s \) parameter also plays an increasing role for large \( r_s \). The idealized theoretical 2DES models ignore layer thickness and impurity effects, and yet seem to be within \( \sim 2\% - 3\% \) of the experimental results for the susceptibility enhancement. The coupled-
The mode form is very successful in capturing the required physics. Thus the QMC, the two-valley CHNC, and the coupled-mode approach based on the one-valley data, provide three independent methods for the study of the strongly coupled 2DES in Si MOSFETs. Finally, we note that the methods used in this paper can be used to study bilayers of electrons and/or holes which are separated by a physical distance $d_L$, the present work being for $d_L=0$.

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