The Correlation Energy and the Spin Susceptibility of the Two-Valley Two-dimensional Electron Gas.

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We find that the spin susceptibility of a two-dimensional electron system with valley degeneracy does not grow critically at low densities, at variance with experimental results [A. Shashkin et al., Phys. Rev. Lett. 96, 036403 (2006)]. We ascribe this apparent discrepancy to the weak disorder present in experimental samples. Our prediction is obtained from accurate correlation energies computed with state-of-the-art diffusion Monte Carlo simulations and fitted with an analytical expression which also provides a local spin density functional for the system under investigation.

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I. INTRODUCTION

The spin properties of low-dimensional electron systems in solid state devices are of great interest in relation to spintronics and quantum computing, both at the fundamental level and for technological applications, the long wavelength spin susceptibility of the two-dimensional electron gas (2DEG) playing an important role in the control of nuclear spins. They are also believed to be intimately related to the apparent metal-insulator transition (MIT) observed in 2D systems in solid state devices.

QMC simulations have provided over the years the method of choice for microscopic studies of the 2DEG, which recently has been shown to provide a rather accurate model for electrons confined in solid state devices. However, no QMC prediction is available for the 2V2DEG and other theoretical estimates, obtained either in RPA or with a classical mapping, do not appear reliable. Here, to calculate the spin susceptibility of the 2V2DEG, we resort to extensive state-of-the-art simulations of the 2V2DEG, using the diffusion Monte Carlo (DMC) technique. We thus obtain for the first time the dependence of the ground state energy on both the density and the spin polarization, also improving on Ref. 9, with the use of twist-averaged boundary conditions (TABC) and trial wavefunctions including backflow (BF).

II. CORRELATION ENERGY OF THE 2V2DEG

In the 2V2DEG electrons possess an additional discrete degree of freedom, i.e., the valley flavor or index, which can be conveniently described with a pseudospin. One may identify electrons with given spin and pseudospin indexes as belonging to a species or component. Accordingly, the paramagnetic 2V2DEG is a four-component system, while both the fully spin-polarized 2V2DEG and the paramagnetic 1V2DEG have two components. For the sake of simplicity, we restrict here to the symmetric case where the number of electrons and the spin polarization are the same for both valleys. Thus, at zero temperature, the state of the system is fully specified by the coupling parameter rs = 1/√π naB and the spin polarization ζ = (n↑−n↓)/n, with n the total electron density, aB the Bohr radius, n↑(↓) the density of up (down) spin electrons. Below, Rydberg units are used throughout.

A. Simulation details

We have performed simulations with the fixed-phase (FP) DMC method, which gives the lowest upper
bound to the ground-state energy consistent with the many-body phase of a suitably chosen, complex-valued trial function. For real trial functions FP-DMC reduces to the standard fixed-node (FN) approximation. A complex trial function allows using TABC, which reduce the size dependence of the kinetic energy by one order of magnitude with respect to periodic boundary conditions (PBC). Furthermore, since TABC do not require closed shells in $k$-space there are no restrictions on the number of electrons per component, so that the polarization can be changed by flipping any number of spins, with fixed total number of electrons. Our trial function is the product of Slater plane-wave (PW) determinants (one per component) and a Jastrow factor. BF correlations are included only for $\zeta = 0$ and $\zeta = 1$, but with FN-DMC and in PBC. Their contribution to the ground-state energy is then added to the PW energies assuming a quadratic dependence on polarization as in Ref. [17]. The ground-state energy per particle $E_N(r_s, \zeta)$, calculated for several values of $r_s$, $\zeta$, and the electron number $N$, is recorded in Table III of Appendix A.

### B. Analytic representation

Following Ref. [17] we determine the energy per particle $E(r_s, \zeta)$ in the thermodynamic limit by fitting to the data listed in Table III an analytic expression which embodies the $r_s$ and $\zeta$ dependence as well as a Fermi-liquid–like size correction:

$$E_N(r_s, \zeta) = E(r_s, \zeta) + \Delta T_N(r_s, \zeta) + (\eta + \eta_s \zeta^2) \frac{1}{r_s N}$$

$$+ (\gamma + \gamma_s \zeta^2) \frac{1}{(r_s N)^{3/2}}.$$  

The fitting parameters $\eta, \eta_s, \gamma$ and $\gamma_s$ take into account potential energy finite-size effects, while $\Delta T_N(r_s, \zeta)$ is the difference of the non-interacting kinetic energy evaluated at finite $N$ with TABC and in the thermodynamic limit. $E(r_s, \zeta)$ is customarily decomposed as sum of the non-interacting kinetic energy, $e_0(r_s, \zeta) = (1 + \zeta^2)/(2r_s^2)$, the exchange energy, $\varepsilon_{x}(r_s, \zeta) = -\frac{4}{3\pi r_s^2}(1+\zeta^{3/2} + (1-\zeta^{3/2})$, and the unknown correlation energy $e_{c}(r_s, \zeta)$, for which we adopt the same analytical representation of Ref. [17].

$$e_c(r_s, \zeta) = (e^{-\beta r_s} - 1)e^{(6)}(r_s, \zeta) + \sum_{i=0.2} \zeta^i \alpha_i(r_s),$$  

where $e^{(6)}(r_s, \zeta) = e_x(r_s, \zeta) - (1 + \frac{3}{128} \zeta^8 + \frac{3}{128} \zeta^8) e_x(r_s, 0)$, and the functions $\alpha_i(r_s)$ are defined by

$$\alpha_i(r_s) = A_i + (B_i r_s + C_i r_s^2 + D_i r_s^3)$$

$$\times \ln \left( 1 + \frac{1}{E_i r_s + F_i r_s^{3/2} + G_i r_s^2 + H_i r_s^3} \right).$$

C. Phase diagram

In Fig. 1 we plot the energies of the paramagnetic and the fully spin-polarized 2V2DEG. They are shown by solid lines labeled with the number of components, $N_c = 4$ and $N_c = 2$, respectively. For comparison, we also plot QMC results for other phases of the 2DEG: $N_c = 1$ labels the fully polarized one-valley 2DEC, whereas the 2D charged-boson fluid corresponds to the limit of an infinite-component 2DEG. The energy of the Wigner crystal is known to be almost independent of the number of components, we report here the result of Ref. [17]. We note that at large $r_s$ as the number of components increases the ground-state energy appears to quickly approach the infinite-component limit.

The dashed line for $N_c = 2$ in Fig. 1 is the result of Ref. [17] for the paramagnetic 2DEG. Its agreement with our curve for the polarized 2V2DEG is expected, but still gratifying: the two calculations differ by details in the extrapolation to the thermodynamic limit, and the closeness of their results supports a good control of the finite-size bias. The dashed line for $N_c = 4$ is instead the result of Ref. [17] for the paramagnetic 2V2DEG. Its difference with the present results conveys a physical information, namely the quantitative effect of BF correlations which were not included in the previous simulations. Backflow improves the nodal structure of the PW wave function, yielding in the FN approximation a tighter upper bound

### Table I: Parameters of the analytic representation

| Parameter | Value | Value | Value |
|-----------|-------|-------|-------|
| $A_i$     | 0.99870 | 0.44570 | 0.0082290 |
| $B_i$     | 15/32(10 - 3\pi) | -0.85288 | 0.048079 |
| $C_i$     | 0.62208 | -7.6202 | 0 |
| $D_i$     | 0.029762 | -1.6194 | -0.051302 |
| $E_i$     | 1.6208 | 12.714 | 25.911 |
| $F_i$     | -0.012856 | 0 | 0 |
| $G_i$     | 0.66150 | 19.692 | 15.072 |
| $H_i$     | 0.029765 | 3.6334 | 6.2334 |
| $\beta$  | 11.879 | | |

The reduced chi square is $\chi^2 = 4.82$. A * marks constrained parameters, whereas $C_2$ is fixed to zero since it turned out to be irrelevant in the fitting procedure. The parameters $\eta, \eta_s, \gamma$ and $\gamma_s$ in Eq. (1) only concern the size extrapolation; their optimal values are 0.056, 0.17, 2.03 and 0.45, respectively.
to the exact ground-state energy \(^{14}\). It is known\(^{17}\) that BF correlations lower the FN energy more for \(N_c = 2\) than for \(N_c = 1\). Here we find that the BF energy gain for \(N_c = 2\) is \({\text{smaller}}\) than for \(N_c = 2\) (see Table \(\ref{table:1}\) of Appendix A), albeit larger than for \(N_c = 1\). The modest effect of BF correlations for \(N_c = 4\) entails only marginal quantitative changes to the phase diagram of the 2V2DEG predicted in Ref. \(\ref{ref:3}\). The density of Wigner crystallization shifts to a slightly lower value, \(r_s \simeq 45\).

Before discussing the spin polarization dependence of the energy and our prediction for the spin susceptibility, we should stress that our results provide the most accurate available estimate for the correlation energy \(\varepsilon_c\) of the 2V2DEG, which in turn is the key ingredient for density functional theory (DFT) studies of inhomogeneous two-valley systems in 2D within the local spin density approximation\(^{28}\). The knowledge of \(\varepsilon_c\) allows also to check the accuracy of the ansatz made in Ref. \(\ref{ref:31}\) to construct the correlation energy of a system with an arbitrary number of components, \(\varepsilon_c(N_c)\), in terms of that of the one valley system\(^{27}\). A comparison between \(\varepsilon_c(N_c)\) from Ref. \(\ref{ref:31}\), the present \(\varepsilon_c\), and the nominally exact QMC results for charged bosons\(^{28}\) (Appendix C) exposes the limited accuracy of \(\varepsilon_c(N_c)\) especially at large \(r_s\), including its prediction\(^{28}\) of an unphysical transition between the nodeless ground state of the infinite-component system and the antisymmetric ground state of the one-component 2DEG. Yet, the comparison between DFT calculations of two-valley symmetric systems using either \(\varepsilon_c(N_c)\) or the present \(\varepsilon_c\) would provide a valuable test of the adequacy of \(\varepsilon_c(N_c)\) for DFT applications.

Our calculations confirm the absence of a transition from the paramagnetic to the fully spin-polarized fluid in the two-valley symmetric system\(^{25}\). Moreover, in the whole density range where the fluid is stable we find no evidence for the stability of a state with partial spin polarization. As illustrated in Fig. \(\ref{fig:1}\) for \(r_s = 25\), \(E(r_s, \zeta)\) displays its minimum at \(\zeta = 0\) and, for all practical purposes, can be considered a convex function of \(\zeta\). Convexity ensures that, by turning on an in-plane magnetic field \(B\), the absolute minimum displayed by the energy goes continuously from \(\zeta = 0\) to \(\zeta = 1\). If the energy exhibits a local maximum or even an inflection point for \(\zeta < 1\), instead, the \(B\)-driven transition to the full spin polarization becomes a first-order one and is accompanied by a jump in the polarization\(^{28}\). This is clearly the case for the 1V2DEG at \(r_s = 25\) also shown in Fig. \(\ref{fig:1}\).

### III. SPIN SUSCEPTIBILITY

The spin susceptibility enhancement\(^{12}\) of the 2V2DEG is readily calculated using Eq. \(\ref{eq:2}\) as

\[
\chi_s/\chi_0 = \left[1 - \frac{2r_s}{\pi} + 2r_s^2\alpha_1(r_s)\right]^{-1}.
\]  

(4)

In Fig. \(\ref{fig:2}\) we compare our QMC prediction with the available experimental results for electrons confined in Si-MOSFETs. It is evident that the 2V2DEG spin susceptibility moderately overestimates experiments at high
density but largely underestimates them at low density, where it does not display any critical growth. In fact $\chi_s$ is a concave function of $r_s$ at all densities where the fluid phase is stable. Indeed, a realistic description of a 2DEG in a solid state device requires consideration of additional elements such as transverse thickness\textsuperscript{18,19} and disorder scattering\textsuperscript{18}. As the thickness is known to suppress the spin susceptibility and a weak disorder to enhance it, at present the only likely candidate to explain the experimentally observed critical behavior of $\chi_s$ appears to be a weak disorder. In Fig. 2 we also report the QMC results of a 1V2DEG\textsuperscript{22}. It is clear that the valley degeneracy causes a substantial suppression of the spin susceptibility, in qualitative agreement with the effect found in experiments on AlAs based quantum wells\textsuperscript{24}, though for an in-plane anisotropic mass. Moreover, $\chi_s(r_s)$ changes from a convex to a concave function in going from the 1V to the 2V2DEG. We also show in the figure the predictions of HF and RPA. The general trend is that, while RPA performs somewhat better than HF, both largely overestimate the QMC predictions and yield divergences which either have no counterpart in QMC, for the 2V2DEG, or in the best case take place at a density about 13 times larger than in QMC, for the 1V2DEG. At least RPA reverts the qualitatively wrong prediction of HF which yields an enhancement of the spin susceptibility in going from the one- to the two-valley system.

IV. DISCUSSION AND CONCLUSIONS

We have reliably estimated the spin susceptibility of the 2V2DEG, which provides the simplest model for electrons confined in Si-MOSFETs. Our results clearly point to the crucial, qualitative role of weak disorder scattering in determining the critical growth found in the measured susceptibility at low density\textsuperscript{20} and to a likely minor, quantitative role of transverse thickness in suppressing the susceptibility at high density. 2D electron systems in high mobility Si-MOSFETs at times have been termed clean, meaning in fact without admixture of local moments\textsuperscript{24}, but also implicitly implying that observed properties would be disorder independent and would correspond to those of an ideally clean electron gas. This latter viewpoint, fostered by the recent experimental observation that the spin susceptibility and a weak disorder to enhance it, at appreciable manner\textsuperscript{18,25}. Moreover, comparing the absolute peak mobilities of Ref. 34 on the one hand and of Ref. 35 on the other, i.e. of systems with quantitatively different length and energy scales (due to different band masses) is not appropriate. If $l$ and $a_B$ are respectively the mean-free path and the effective Bohr radius in a given system, we find that the peak of $l/(r_s a_B)$ for the EG of Ref. 34 is only 3 times smaller than that of the EG of Ref. 35. Hence the experiment in Ref. 34 in our opinion is not at all conclusive in ruling out an effect of disorder on the effective mass, let alone on the spin susceptibility of these systems.

We have also obtained: an assessment of the backflow effects on the energy of the two-valley paramagnetic phase, which remains stable with respect to any partially or fully polarized phase, up to the Wigner crystallization; an analytical fit of the QMC correlation energy, which also interpolates between exact high and low-density limits, and provides a local spin density functional for DFT studies of two-valley systems; the clear indication that an accurate account of correlation beyond RPA is crucial when considering the properties of both the 1V- and 2V2DEG.

APPENDIX A: DETAILS OF THE DMC SIMULATIONS

The trial function was chosen of the usual Slater-Jastrow form, $\Psi(R) = D(R) J(R)$, where $R \equiv (r_1, \ldots, r_N)$ represents the coordinates of the $N$ electrons. The Jastrow factor is a pair product, $J(R) = \exp \left[ - \sum_{i<j} u(r_{ij}) \right]$, with $u(r)$ the parameter-free RPA pseudopotential\textsuperscript{15}. The phase structure is fixed by the complex factor $D = \prod_u D_u$, i.e., a product of Slater determinants, one for each spin-valley component.

Most of the simulations were carried out with the standard plane-wave (PW) choice for the one-particle orbitals, $D^{\text{PW}}_\nu = \det \{ \exp(\hat{\mathbf{k}} \cdot \mathbf{r}_i) \}$. For $\zeta = 0$ and $\zeta = 1$ we also included backflow (BF) correlations\textsuperscript{15}, $D^\eta = \det \{ \exp(\hat{\mathbf{k}}_1 \cdot \mathbf{x}_j) \} \equiv \det \{ \exp(\hat{\mathbf{k}}_1 \cdot \mathbf{x}_j) \} \exp(-\sum_{i<j} \eta(r_{ij}))$, where $\mathbf{x}_1 = \mathbf{r}_i + \sum_{j} \eta(r_{ij}) (\mathbf{r}_i - \mathbf{r}_j)$ and the BF function $\eta(r)$ (of the form suggested in\textsuperscript{15}) was optimized by minimization of the variational energy.

We simulated the imaginary-time evolution of the system by a branching random walk, using a short-time approximation of the importance-sampled Green’s function and exerting control on the number of walkers. Calculations were performed at $r_s = 1, 2, 5, 10, 20, 40$. For $\zeta = 0$ and $\zeta = 1$ we chose several values of the number of electrons between $N = 36$ and $N = 116$, whereas 11 intermediate values of the polarization, defined by flipping one spin at a time, were studied for $N = 52$. The twist average, for the PW simulations, was performed on a mesh defined by $q_x(i) = (i-1/2)/\Delta, q_y(j) = \Delta(j-1/2), 1 \leq i \leq 8, i \leq j \leq 8, \Delta = \pi/8 L$, with $L$ the side of the simulation box. Long-range interactions were dealt with the optimized-splitting method of Ref. 57.

Extrapolation to zero time step $\tau$ and infinite number
TABLE II: Difference $\Delta = E^{BF}_N (r_s, \zeta) - E^{PW}_N (r_s, \zeta)$ between the BF and the PW energy (in Rydberg per particle) at selected values of $r_s$, $\zeta$, $N$. In parentheses the statistical error on the last digit.

| $r_s$ | $N$ | $\zeta = 0$ |  | $\zeta = 1$ |  |
|-------|-----|-------------|---|-------------|---|
|       |     | $\Delta$    | b| $\Delta$    | b|
| 1     | 52  | -0.0028(1)  |   | 50 -0.0034(1) |   |
|       | 58  | -0.0035(2)  |   | 50 -0.0032(1) |   |
| 2     | 52  | -0.00166(5) |   | 42 -0.00175(9)|   |
|       | 50  | -0.00192(9) |   | 50 -0.00192(9)|   |
| 5     | 52  | -0.00057(2) |   | 50 -0.00077(3)|   |
|       | 58  | -0.00088(3) |   | 58 -0.00088(3)|   |
| 10    | 52  | -0.00021(1) |   | 42 -0.00025(1)|   |
|       | 84  | -0.00030(2) |   | 50 -0.00030(2)|   |
|       | 58  | -0.00032(2) |   | 58 -0.00032(2)|   |
| 20    | 52  | -0.000043(6)|   | 42 -0.000081(7)|   |
|       | 50  | -0.000085(7)|   | 50 -0.000085(7)|   |
| 40    | 52  | -0.000020(1)|   | 50 -0.000020(1)|   |

APPENDIX B: HIGH AND LOW DENSITY LIMIT OF THE CORRELATION ENERGY OF THE FOUR COMPONENT 2DEG

We directly refer to Ref. [17] for both the $r_s \to \infty$ limit, whose leading terms in $r_s^{-1}$ and $r_s^{-3/2}$ are independent of the number of components [38], and the $r_s \to 0$ limit at $\zeta = 1$, which is the same two-component system as the one-valley case at $\zeta = 0$ [17].

Here we only need to specify the high-density limit for the four-component system, $\lim_{r_s \to 0} e_c (r_s, 0) = A_0 + B_0 r_s \ln r_s$. Generalizing the procedure of Ref. [39] to the multivalley case, we write $e_c$ as the sum of the second-order exchange energy $e_2^{(c)}$ and the ring contribution $e_c^{(r)}$, whose lowest order $e_c^{(r)}$ is the direct term of the second-order energy per particle. It turns out that $e_2^{(c)}$ is a constant, independent of $r_s$ and the number of components of the system, $N_c$, while $e_c^{(r)} (r_s, N_c) \propto N_c f(r_s N_c^{3/2})$, so that the following scaling law holds

$$e_c^{(r)} (r_s, 4) = 2e_2^{(c)} (4\sqrt{2} r_s, 2).$$

By applying the scaling law (B1) to the leading terms of $e_c$, we find $A_0 = e_2^{(b)} + 2e_2^{(r)} (2) = -0.99870$, $B_0 = 16 (10 - 3\pi)/(3\pi)$.

APPENDIX C: CHECK OF AN APPROXIMATE MULTICOMPONENT CORRELATION ENERGY

In Fig. 3 we show a comparison between the multicomponent correlation energy $\tilde{\epsilon}_c (N_c)$ of Ref. [31] and various simulation results, including the present two-valley calculation, and the nominally exact QMC results for charged bosons [38]. Total energies are displayed. The scale of the figure, emphasizes the limited accuracy of $\tilde{\epsilon}_c (N_c)$ in the large $r_s$ regime.

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TABLE III: Data used for the fit described in the paper. Twist-averaged DMC energy in Rydberg per particle \( E_N(r_s, \zeta) \), calculated at finite \( N \), extrapolated to zero time step and infinite number of walkers, and including BF correlations; in parentheses the statistical error on the last two figures shown. The backflow correction was obtained from Table II employing the results at the largest \( N \) available.

| \( r_s \) | \( N \) | \( \zeta \) | \( E_N(r_s, \zeta) \) | \( r_s \) | \( N \) | \( \zeta \) | \( E_N(r_s, \zeta) \) | \( r_s \) | \( N \) | \( \zeta \) | \( E_N(r_s, \zeta) \) |
|-------|-------|-------------|-----------------|-------|-------|-------------|-----------------|-------|-------|-------------|-----------------|
| 1     | 36    | 0           | -0.76940(15)    | 5     | 36    | 0           | -0.308540(26)   | 20    | 36    | 0           | -0.0930324(80)  |
| 1     | 36    | 1           | -0.4250(21)     |       | 36    | 1          | -0.299849(46)   |       | 36    | 1          | -0.092705(13)   |
| 52    | 0     | -0.76418(14)|                  | 52    | 0     | -0.308001(25) |                  | 42    | 1       | -0.092681(13)|
| 52    | 1/13  | -0.76192(14)|                  | 52    | 1/13  | -0.307933(26) |                  | 52    | 0       | -0.0925907(79)|
| 52    | 2/13  | -0.75430(15)|                  | 52    | 2/13  | -0.307727(26) |                  | 52    | 1/13   | -0.0928559(80)|
| 52    | 3/13  | -0.74537(15)|                  | 52    | 3/13  | -0.307614(27) |                  | 52    | 2/13   | -0.0929483(81)|
| 52    | 4/13  | -0.73040(15)|                  | 52    | 4/13  | -0.307191(28) |                  | 52    | 3/13   | -0.0929498(83)|
| 52    | 5/13  | -0.71189(16)|                  | 52    | 5/13  | -0.306660(29) |                  | 52    | 4/13   | -0.0929340(85)|
| 52    | 6/13  | -0.68872(16)|                  | 52    | 6/13  | -0.305994(31) |                  | 52    | 5/13   | -0.0929046(87)|
| 52    | 7/13  | -0.66258(17)|                  | 52    | 7/13  | -0.305416(33) |                  | 52    | 6/13   | -0.0928788(91)|
| 52    | 8/13  | -0.63301(17)|                  | 52    | 8/13  | -0.304745(35) |                  | 52    | 7/13   | -0.0928363(96)|
| 52    | 9/13  | -0.59922(18)|                  | 52    | 9/13  | -0.303896(37) |                  | 52    | 8/13   | -0.0928420(10)|
| 52    | 10/13 | -0.55906(19)|                  | 52    | 10/13 | -0.302872(39) |                  | 52    | 9/13   | -0.092816(11)|
| 52    | 11/13 | -0.51827(19)|                  | 52    | 11/13 | -0.301915(42) |                  | 52    | 10/13  | -0.09275(11)|
| 52    | 12/13 | -0.47881(21)|                  | 52    | 12/13 | -0.300624(46) |                  | 52    | 11/13  | -0.092735(12)|
| 84    | 0     | -0.76258(14)|                  | 84    | 0     | -0.307778(25) |                  | 84    | 1     | -0.0926590(13)|
| 84    | 1     | -0.42201(21)|                  | 84    | 1     | -0.299197(45) |                  | 84    | 0     | -0.0929138(79)|
|       |       |             |                  |       |       |             |                  |       | 100    | 1     | -0.092557(13)|
|       |       |             |                  |       |       |             |                  |       | 84     | 1     | -0.092562(13)|

\( N \) \( r_s \) \( N \) \( \zeta \) \( E_N(r_s, \zeta) \) \( N \) \( \zeta \) \( E_N(r_s, \zeta) \) \( N \) \( \zeta \) \( E_N(r_s, \zeta) \)

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Indeed, for the one-valley 2DEG the RPA grossly overestimates \( \chi_s \) and predicts a divergence at moderate low-density which can only be ascribed to its limited accuracy. Similarly, a small but unjustified change of the correlation energy in the calculations carried out for the 2V2DEG within the classical mapping changes a \( \chi_s \) finite and smooth at all densities in a diverging one.

Evidently, we disregard the valley splitting predicted when going beyond the effective mass approximation.

The coefficients of the leading powers of \( r_s \) are kept fixed to their analytical values for the crystal phase in Ref. 17, whereas they are fitting parameters in the present work. Further energy gain for the four-component phase could be in principle obtained by allowing spin/valley contamination: i.e. considering a spin/valley dependent backflow. However, a systematic study exploiting this possibility for the unpolarized three-dimensional electron gas gave energies in error bar with ones obtained with spin-independent backflow.

The convexity of \( E(\mu_s, \zeta) \) is spoiled by the exchange term at some finite polarization \( \zeta_c \). However, for \( r_s \gtrsim 1 \), correlation effects push \( \zeta_c \) exponentially close to 1, in a range \( 1 - \zeta_c \propto e^{-\beta r_s} \).

The coefficients of the leading powers of \( r_s \) are kept fixed to their analytical values for the crystal phase in Ref. 17, whereas they are fitting parameters in the present work.