Itinerant–electron magnetism: the importance of many-body correlations

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Do electrons become ferromagnetic just because of their repulsive Coulomb interaction? Our calculations on the three-dimensional electron gas imply that itinerant ferromagnetism of delocalized electrons without lattice and band structure, the most basic model considered by Stoner, is suppressed due to many-body correlations as speculated already by Wigner, and a possible ferromagnetic transition lowering the density is precluded by the formation of the Wigner crystal.

In 1929, Felix Bloch addressed the possibility of itinerant ferromagnetism,\(^1\) where the same electrons forming the conducting state give also rise to ferromagnetism. Considering the free homogeneous electron gas (jellium) as a minimal model to describe electrons in a metal, he concluded that the exchange energy may lead to a ferromagnetic state at densities slightly below those occurring in alkali metals. Considering correlation between positions of electrons with antiparallel spin, Wigner\(^\pi\) approximately calculated the correlation energy—the gain of energy compared to the Hartree–Fock approximation—and pointed out the possibility of crystalline order at low densities. In the same paper, he also anticipated that the magnitude of the correlation energy is important for questions of para– and ferromagnetism modifying Bloch’s theory on itinerant magnetism. Later, Stoner\(^4\) predicted the occurrence of a continuous transition between zero and full magnetization at zero temperature introducing a repulsive energy term between opposite spin electrons to phenomenologically account for correlation effects. The threshold of the ratio between this repulsive interaction constant and the Fermi energy, is now commonly known as Stoner criterium.

In this paper, we show that Stoner’s instability is precluded by the transition to the Wigner crystal and argue that itinerant magnetism is quite generally suppressed by correlation effects in the ground state of homogeneous quantum fluids with spin–independent repulsive interactions.

Starting from Bloch’s prediction, based on the Hartree–Fock approximation, of ferromagnetism at \(r_s \equiv a/a_B > 5.45\), where \(a_B\) is the Bohr radius and \(a = (4\pi n/3)^{-1/3}\) is the mean electron distance at density \(n\), more accurate calculations taking better into account electron correlations, notably based on quantum Monte Carlo methods, have shifted the expected magnetic transition in the three dimensional electron gas model towards significantly lower densities.\(^11,12\) The most recent quantum Monte Carlo calculations\(^13\) support Stoner’s picture of a continuous magnetic transition, with the onset of partial spin polarization at \(r_s \approx 50\) and completion of full polarization at \(r_s \approx 100\), just before Wigner crystallization which is estimated to occur at \(r_s = 106(1)\) in Ref.\(^10\).

We present new results based on a sequence of wave functions featuring iterative backflow transformations\(^11,12\) within the variational (VMC) and the more accurate fixed-phase diffusion (DMC) Monte Carlo methods.\(^13\) Zero–variance extrapolation\(^11\) of the ground state energies at finite system size allows us to reliably control the remaining, systematic bias of the fixed-phase DMC calculations. Finite size corrections due to single-particle shell effect\(^15\) and two-body terms\(^16,17\) are applied for thermodynamic limit extrapolation. Improved accuracy proves crucial, as our calculations show that many-body correlations of the ground state wave function favor the unpolarized phase of the electron liquid compared to partial or fully polarized states and eventually prevent itinerant magnetism in jellium at any densities above crystallization. We also update the density of the transition to the Wigner crystal to a slightly lower value, \(r_s = 113\).

In the following, we describe the details of our numerical methods to determine the low-density ground state phase diagram of jellium—non-relativistic electrons interacting via Coulomb’s potential with each other and with a homogeneous positive background to guarantee charge neutrality.\(^13,19\) The ground state energy per electron of the model at three values of the electronic density, \(n\), corresponding to \(r_s = 70, 100,\) and \(120\), and five different spin-polarization, \(\zeta (\zeta = 0.0, 0.42, 0.61, 0.79, 1.0)\), is addressed by variational and diffusion Monte Carlo simulation\(^13\) of a finite system containing \(N = 66\) electrons imposing periodic boundary conditions for the particles’ positions; the long-range Coulomb potential is evaluated by standard splitting into real and reciprocal space contributions.\(^20,21\)

In the DMC runs, the number of walkers is 1280 and the time step is 15, 20 and 30 \(\text{Ry}^{-1}\) for \(r_s = 70, 100\) and 120 respectively. The estimated time step error is \(10^{-7}\) \(\text{Ry}\) or less, which is about the size of the statistical error on our final results (the zero–variance extrapolation of the DMC energy, see below). The population control bias is even smaller, of the order of \(10^{-3}\) \(\text{Ry}\).
tem is limited by the underlying many-body trial wave function \( \Psi \) used for calculating expectation values in VMC\(^{13} \) and for imposing the phase in DMC\(^{14} \) respectively. In order to remove such a bias, we consider a series of trial wave functions of increasing quality, starting from the standard Jastrow–Slater and backflow forms (PW and BF\(^{12} \)) and adding up to four iterative backflow transformations (BF\(_1\), ..., BF\(_4\))\(^{11} \).

Specifically, the Jastrow-Slater wave function PW(\( \mathbf{R} \)) explicitly depends on the coordinates \( \mathbf{R} \) of all the particles through two-body and three-body pseudopotentials \( u_0 \) and \( \xi_0 \) in the Jastrow factor \( \exp(-U_0(\mathbf{R})) \), and through plane–wave orbitals in the Slater determinant \( D(\mathbf{R}) \). We then recursively build sets of transformed coordinates \( Q_0, ..., Q_k \), where \( Q_i \) depends on \( Q_{i-1} \) through the \( i \)-th backflow pseudopotential \( \eta_i \), with \( Q_{-1} \equiv \mathbf{R} \). The \( k \)-th iterative backflow wave function is

\[
\text{BF}_k(\mathbf{R}) = \exp(-U_0(Q_{-1}) + \ldots + U_k(Q_{k-1}))D(Q_k). \tag{1}
\]

In this work we include both two- and three-body pseudopotentials \( u_0 \) and \( \xi_0 \) in \( \exp(-U_0) \), and only two-body pseudopotentials \( u_i \) in \( \exp(-U_i) \) for \( i = 1, ..., k \). The plane–wave orbitals in the Slater determinant are evaluated at the last set of transformed coordinates, \( Q_k \).

The two-body pseudopotential \( u_0 \) is initially of the the RPA form\(^{15} \) with an explicit long-range part in Fourier space spanning the first 20 shells of reciprocal vectors, and the real-space part represented by locally piecewise-quintic Hermite interpolants (LPQHI) with 8 degrees of freedom which are subsequently treated as optimization parameters. The three-body pseudopotential \( (\xi_0) \), the backflow pseudopotentials \( (\eta_i \text{ with } i = 0, \ldots, k) \), and the two-body pseudopotentials \( (u_i \text{ with } i = 1, \ldots, k) \) are all expressed as LPQHI with 6 degrees of freedom each, with the exception of \( \eta_0 \) which is augmented with 5 shells of Fourier components. The LPQHI coefficients of all the pseudopotentials, as well as the Fourier components of \( \eta_0 \), are optimized independently for each wave function in the hierarchy.

The energy \( E \) computed for \( r_s = 100 \) in VMC and DMC simulations using all the above wave functions is plotted in Fig. 1 against the corresponding VMC variance \( \sigma^2 = \langle \Psi | (H - \langle \Psi | H | \Psi \rangle)^2 | \Psi \rangle \). The exact ground–state energy, which has zero variance, can be reliably estimated by extrapolation\(^{11} \), given the smoothness of the data over a significant range extending to very low values of \( \sigma^2 \). We assume a quadratic dependence of \( E \) on \( \sigma^2 \). Since the range of validity of such a dependence is not known, we perform the extrapolation with and without the highest energies and variances, obtained with the PW wave function. The result does not change significantly if we include the PW result and/or switch between VMC and DMC data for the extrapolation. In particular, Figure 2 shows that the polarization energy is only marginally influenced by the choice of the data set.

Twist-averaged boundary conditions of the trial wave function\(^{15} \) on a regular grid of 1000 twist angles are used to reduce shell effects of the finite simulation cell and avoid thermodynamic limit extrapolation without resorting to large simulation cells. Residual single particle shell effects due to the discrete twist grid and to reduced-symmetry open-shell fillings for finite polarizations with \( N = 66, \Delta T_0 \), are estimated from the non-interacting electron gas. Two–particle finite size corrections for the potential and kinetic energy, \( \Delta FSE \), are addressed by interpolation of the long–range part of the static structure factor and by the analytical long–range expressions for the two–body and backflow pseudopotentials \( u_0 \) and \( \eta_0 \) of the wavefunction\(^{12} \). At low densities, the corrections \( \Delta FSE \) are largely dominated by the zero–point energy of the plasmon\(^{16} \). Whereas the single particle size corrections depend on the spin polarization, the long–range structure factor does not reveal any systematic dependence on \( \zeta \) within the statistical error of the present simulations. Therefore, we average the structure factor over spin–polarizations in the calculation of \( \Delta FSE \), so that the final polarization energy is not affected by statistical fluctuations in the estimates of \( \Delta FSE \). Only the absolute value of the estimated ground state energy, used below to locate the Wigner crystallization, is then susceptible to the details of the calculation of \( \Delta FSE \).

The results for the energies and the variances obtained with different trial wave functions, the zero–variance extrapolations, and the finite–size corrections are collected in the Supplemental Material\(^{22} \). Note that the variance extrapolation is done on the energies of the finite–size system, and size corrections (for the polarization energy and the Wigner crystallization) are applied afterwards.

The final polarization energy of jellium at low densities, our main result, is shown in Fig. 3 for \( r_s = 70, 100 \) and 120. It is obtained from the zero–variance extrapolation of the DMC energy, excluding the PW result. This choice gives the smoothest polarization energy, as well as the lowest \( \chi^2 \) in the fit to the energy vs. variance data, but it is otherwise uninfluential for the conclusion that \( E(\zeta) \) is higher than \( E(0) \) for all the densities considered, and therefore a partially or fully polarized state is never stable.

The zero–variance extrapolation of the DMC energy, corrected for finite–size effects, is compared in Fig. 4 with the fixed–node DMC energy\(^{15} \) of the Wigner crystal of Ref.\(^{10} \) as a function of \( r_s \). For the crystal phase, finite–size effects are assessed using large simulation cells with up to 512 electrons\(^{19} \). This procedure differs from that used in the present work for the liquid phase, but it should be equally reliable. The fixed–node DMC bias\(^{17} \) for the crystal phase is negligible: it is bounded by (and presumably much smaller than) the difference between the fixed–node energy and the exact bosonic ground–state energy, which we find to be of the order of the statistical error on the crystal data of Fig. 4. The critical value for the Wigner crystallization is shifted to \( r_s = 113(1) \).

In this paper, we have presented accurate quantum Monte Carlo calculations addressing the possibility of a magnetically polarized fluid in the ground state phase diagram of the homogeneous electron gas. We have shown
FIG. 1. Extrapolation of the energy to zero variance for \( r_s = 100 \) at polarizations \( \zeta = 0 \) and 1. The data are calculated with with VMC and DMC using PW, BF0, ... , BF4 wave functions in order of decreasing energy. The reference value \( \sigma_0^2 \) is the variance of the local energy at \( \zeta = 0 \) with the PW wave function. The curves are quadratic fits; for each set of data points (VMC and DMC for \( \zeta = 1 \) and 2) there are two curves, one of which excludes the PW energy from the fit.

FIG. 2. The polarization energy \( E(\zeta) - E(0) \) obtained from zero–variance extrapolations of the VMC and DMC energies, with or without the PW result. The common reference energy \( E_0 \) is the zero–variance extrapolation without the PW result of the DMC value \( E(\zeta = 0) \).

FIG. 3. The polarization energy \( E(\zeta) - E(0) \) obtained from zero–variance extrapolations of the DMC energies without the PW result. The lines are polynomial fits with terms of order 0, 2 and 6.

FIG. 4. DMC energy as a function of \( r_s \) for the paramagnetic and the ferromagnetic fluid and for the Wigner crystal. The arrow at \( r_s = 113 \) locates the crystallization point.

that iterated backflow wave functions\(^{11,12}\) provide highly accurate results for the energy and very low values of its variance, such that a zero variance extrapolation provides fairly unbiased results for the polarization energy. Our calculations clearly demonstrate that the simple mean-field picture based on Stoner’s model is not sufficient to explain itinerant ferromagnetism as the partially or fully polarized fluid state is unstable versus Wigner crystallization.

Therefore, in addition to repulsive interparticle interactions, band structure effects must play an essential role for the occurrence of itinerant ferromagnetism in real materials.

Similar results have been found for liquid \(^3\)He in two\(^{11,123}\) and three dimensions\(^{12,124}\), the two dimensional electron gas\(^{20}\), and two dimensional quantum gases with repulsive dipolar interaction\(^{20}\), where accurate, quantitative treatment of correlation effects have always stabili-
lized the spin-unpolarized phase.

From a more general point of view, Stoner’s instability constitutes a reconstruction of the Fermi surface of the unpolarized to the polarized gas due to interactions. However, this instability is quite naturally in competition with the reconstruction of the Fermi surface related to spin and charge density waves (not addressed in this work) or Brillouin zone formation for Wigner crystallization. Despite the quite different interparticle interaction, hard or soft core potentials, the Stoner transition to a spin-polarized phase predicted within mean-field arguments seems to be quite generally preceded by transition to a crystalline phase for homogeneous systems with spin-independent interactions.

Recent experimental efforts have been devoted to realize Stoner’s model within ultracold atomic gases, where the interaction between two fermions is essentially described by momentum and energy independent s-wave scattering. However, there, the strong repulsive s-wave interaction is intrinsically connected with a short range interparticle bound state leading to molecule formation. Although local spin-correlations have been observed, the interpretation of the experimental observations is not straightforward.

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1 F. Bloch, Zeitschrift f. Physik 57, 545 (1929).
2 E. P. Wigner, Phys. Rev. 46, 1002 (1934).
3 E. P. Wigner, Trans. Farad. Soc. 34, 678 (1938).
4 E.C. Stoner, Proc. R. Soc. Lond. A 165, 372 (1938).
5 D. Ceperley, Phys. Rev. B 18, 3126 (1978).
6 D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. 45, 566 (1980).
7 D. M. Ceperley and B. J. Alder, Journal de Physique C7, 295 (1980).
8 G. Ortiz, M. Harris, and P. Ballone, Phys. Rev. Lett. 82, 5317 (1999).
9 F. H. Zong, C. Lin, and D. M. Ceperley, Phys. Rev. E 66, 036703 (2002).
10 N. D. Drummond, Z. Radnai, J. R. Trail, M. D. Towler, and R. J. Needs, Phys. Rev. B 69, 085116 (2004).
11 M. Taddei, M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. B 91, 115106 (2015).
12 M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. Lett. 120, 205302 (2018).
13 L.K. Wagner and D.M. Ceperley, Rep. Prog. Phys. 79, 094501 (2016).
14 G. Ortiz, D.M. Ceperley, and R.M. Martin, Phys. Rev. Lett. 71, 2777 (1993).
15 C. Lin, F.-H. Zong, and D. M. Ceperley, Phys. Rev. E 64, 016702 (2001).
16 S. Chiesa, D.M. Ceperley, R.M. Martin, and M. Holzmann, Phys. Rev. Lett. 97, 076404 (2006).
17 M. Holzmann, R.C. Clay III, M. A. Morales, N.M. Tubman, D. M. Ceperley, and C. Pierleoni, Phys. Rev. B 94, 035126 (2016).
18 G. F. Giuliani and G. Vignale, Quantum Theory of the Electron Liquid (Cambridge University Press, Cambridge, 2005).
19 R.M. Martin, L. Reining, and D. M. Ceperley, Interacting Electrons, Cambridge University Press, Cambridge (2016).
20 P.P. Ewald, Ann. Phys. 64, 253 (1921).
21 V. Natoli and D.M. Ceperley, J. Comput. Phys. 117, 171 (1995).
22 See Supplemental Material at [http://link] for VMC and DMC data, zero–variance extrapolations, and finite–size corrections.
23 M. Nava, A. Motta, D. E. Galli, E. Vitali, and S. Moroni, Phys. Rev. B 85, 184401 (2012).
24 M. Holzmann, B. Bernu, and D.M. Ceperley, Phys. Rev. B 74, 104510 (2006).
25 N. D. Drummond and R. J. Needs Phys. Rev. Lett. 102, 126402 (2009).
26 T. Comparin, R. Bombin, M. Holzmann, F. Mazzanti, J. Boronat, and S. Giorgini, Phys. Rev. A 99, 043609 (2019).
27 A. W. Overhauser, Phys. Rev. Lett. 4, 462 (1960); Phys. Rev. 128, 1437 (1962).
28 F. Delyon, B. Bernu, L. Baguet, and M. Holzmann, Phys. Rev. B 92, 235124 (2015).
29 D. Gontier, C. Hainzl, and M. Lewin, Phys. Rev. A 99, 052501 (2019).
30 G.-B. Jo1, Y.-R. Lee, J.-H. Choi, C. A. Christensen, T. H. Kim, J. H. Thywissen, D. E. Pritchard, W. Ketterle, Science 325, 1521 (2009).
31 G. Valtolina, F. Scazza, A. Amico, A. Burchianti, A. Recati, T. Enss, M. Inguscio, M. Zaccanti, and G. Roati, Nature Physics 13, 704 (2017).
SUPPLEMENTAL MATERIAL

This supplemental materials contains tables with all the finite–size energies and variances for different wave functions, densities and polarizations as specified in the main text, as well as zero–variance extrapolations and finite–size corrections.
| ζ  | Ψ       | $\sigma^2/\sigma_0^2$ | VMC          | DMC          | $\Delta T_0$ | $\Delta FSE$ |
|-----|---------|------------------------|--------------|--------------|-------------|-------------|
| 0.00| PW      | 1.00000(326)           | -21.17385(39) | -21.31364(28) | -0.00106    | 0.04373     |
|     | BF0     | 0.32706(91)            | -21.31461(21) | -21.35302(12) | -0.00106    | 0.04079     |
|     | BF1     | 0.15819(51)            | -21.34883(12) | -21.36427(07) | -0.00106    | 0.04097     |
|     | BF2     | 0.07838(25)            | -21.36009(08) | -21.36794(08) | -0.00106    | 0.04117     |
|     | BF3     | 0.07079(28)            | -21.36121(08) | -21.36841(03) | -0.00106    | 0.04180     |
|     | BF4     | -                     | -            | -            | -            | -            |
| ext full |       | -21.37267(160)        | -21.37238(56) |              |             |             |
| ext w/o PW |     | -21.36843(48)        | -21.37090(26) |              |             |             |
| 0.42 | PW      | 0.96797(304)           | -21.18668(40) | -21.31704(29) | -0.00053    | 0.04373     |
|     | BF0     | 0.30709(89)            | -21.31742(19) | -21.35256(09) | -0.00053    | 0.04079     |
|     | BF1     | 0.13848(48)            | -21.34880(12) | -21.36240(06) | -0.00053    | 0.04097     |
|     | BF2     | 0.08538(28)            | -21.35469(09) | -21.36481(08) | -0.00053    | 0.04117     |
|     | BF3     | 0.07069(30)            | -21.35860(08) | -21.36555(04) | -0.00053    | 0.04180     |
|     | BF4     | -                     | -            | -            | -            | -            |
| ext full |       | -21.37013(102)        | -21.36941(38) |              |             |             |
| ext w/o PW |     | -21.36710(32)        | -21.36832(19) |              |             |             |
| 0.61 | PW      | 0.91064(303)           | -21.19929(46) | -21.32103(23) | -0.00066    | 0.04373     |
|     | BF0     | 0.28858(86)            | -21.32023(18) | -21.35184(07) | -0.00066    | 0.04079     |
|     | BF1     | 0.13152(42)            | -21.34817(10) | -21.36046(06) | -0.00066    | 0.04097     |
|     | BF2     | 0.08425(28)            | -21.35481(09) | -21.36249(04) | -0.00066    | 0.04117     |
|     | BF3     | 0.06870(56)            | -21.35706(09) | -21.36316(03) | -0.00066    | 0.04180     |
|     | BF4     | -                     | -            | -            | -            | -            |
| ext full |       | -21.36794(97)        | -21.36678(32) |              |             |             |
| ext w/o PW |     | -21.36515(49)        | -21.36563(13) |              |             |             |
| 0.79 | PW      | 0.81174(275)           | -21.21608(37) | -21.32436(25) | -0.00074    | 0.04373     |
|     | BF0     | 0.26009(70)            | -21.32214(17) | -21.34939(14) | -0.00074    | 0.04079     |
|     | BF1     | 0.12528(34)            | -21.34817(10) | -21.36046(06) | -0.00074    | 0.04097     |
|     | BF2     | 0.08368(27)            | -21.35111(07) | -21.35773(05) | -0.00074    | 0.04117     |
|     | BF3     | 0.06924(48)            | -21.35314(07) | -21.35856(03) | -0.00074    | 0.04180     |
|     | BF4     | -                     | -            | -            | -            | -            |
| ext full |       | -21.36358(80)        | -21.36170(40) |              |             |             |
| ext w/o PW |     | -21.36116(44)        | -21.36097(96) |              |             |             |
| 1.00 | PW      | 0.63694(203)           | -21.23829(34) | -21.32189(21) | -0.00066    | 0.04373     |
|     | BF0     | 0.21696(58)            | -21.31933(16) | -21.34051(07) | -0.00066    | 0.04079     |
|     | BF1     | 0.10935(31)            | -21.33719(09) | -21.34574(04) | -0.00066    | 0.04097     |
|     | BF2     | 0.07083(24)            | -21.34198(08) | -21.34700(05) | -0.00066    | 0.04117     |
|     | BF3     | 0.05861(16)            | -21.34384(07) | -21.34774(05) | -0.00066    | 0.04180     |
|     | BF4     | -                     | -            | -            | -            | -            |
| ext full |       | -21.35177(67)        | -21.35030(40) |              |             |             |
| ext w/o PW |     | -21.35006(112)       | -21.34945(77) |              |             |             |

TABLE I. Energy per particle (in mRy) at various spin polarizations ζ for $r_s = 70$ from VMC and DMC simulations of 66 electrons in twist-averaged boundary conditions using different wave functions; variance of the local energy relative to that of the PW wave function at ζ = 0, $\sigma^2/\sigma_0^2$; zero–variance extrapolation of the VMC and DMC energies with or without the PW result; finite size errors for the discretization of k-space through the non–interacting shell effect, $\Delta T_0$, and through integrals involving the static structure factor, $\Delta FSE$ (the latter uses the RPA two–body pseudopotential and the analytic backflow; it is averaged over the polarizations because there is not enough statistical precision to detect a polarization dependence).
| $\zeta$ | $\Psi$ | $\sigma^2/\sigma_0^2$ | VMC | DMC | $\Delta T_0$ | $\Delta F_{\text{SE}}$ |
|-------|-------|----------------|------|------|-------------|----------------|
| 0.00  | PW    | 1.00000(232)  | -15.25228(13) | -15.35243(28) | -0.00052 | 0.02543 |
|       | BF0   | 0.34206(80)   | -15.34443(13) | -15.37588(09) | -0.00052 | 0.02382 |
|       | BF1   | 0.15445(43)   | -15.37101(08) | -15.38345(07) | -0.00052 | 0.02413 |
|       | BF2   | 0.09342(23)   | -15.37899(06) | -15.38588(03) | -0.00052 | 0.02414 |
|       | BF3   | 0.07226(17)   | -15.38112(05) | -15.38661(03) | -0.00052 | 0.02441 |
|       | BF4   | 0.06484(17)   | -15.38189(04) | -15.38683(04) | -0.00052 | 0.02468 |
|       | ext full |           | -15.39050(57) | -15.38953(13) |            |               |
|       | ext w/o PW |         | -15.38866(59) | -15.38914(17) |            |               |
| 0.42  | PW    | 0.91178(131)  | -15.26052(11) | -15.35652(30) | -0.00026 | 0.02543 |
|       | BF0   | 0.32012(77)   | -15.34784(12) | -15.37672(08) | -0.00026 | 0.02382 |
|       | BF1   | 0.14920(24)   | -15.37188(06) | -15.38343(06) | -0.00026 | 0.02413 |
|       | BF2   | 0.09047(25)   | -15.37929(06) | -15.38558(03) | -0.00026 | 0.02414 |
|       | BF3   |            |                 |                 |            |               |
|       | BF4   | 0.06415(18)   | -15.38196(05) | -15.38645(03) | -0.00026 | 0.02468 |
|       | ext full |           | -15.39015(69) | -15.38899(16) |            |               |
|       | ext w/o PW |         | -15.38876(64) | -15.38857(09) |            |               |
| 0.61  | PW    | 0.89692(241)  | -15.26984(24) | -15.35928(33) | -0.00032 | 0.02543 |
|       | BF0   | 0.30266(85)   | -15.35090(12) | -15.37749(10) | -0.00032 | 0.02382 |
|       | BF1   | 0.14164(46)   | -15.37289(07) | -15.38338(06) | -0.00032 | 0.02413 |
|       | BF2   | 0.08791(24)   | -15.37626(05) | -15.38536(04) | -0.00032 | 0.02414 |
|       | BF3   | 0.07001(65)   | -15.38172(15) | -15.38582(03) | -0.00032 | 0.02441 |
|       | BF4   |            |                 |                 |            |               |
|       | ext full |           | -15.39009(58) | -15.38846(13) |            |               |
|       | ext w/o PW |         | -15.38857(62) | -15.38811(21) |            |               |
| 0.79  | PW    | 0.81249(241)  | -15.28176(22) | -15.36306(23) | -0.00036 | 0.02543 |
|       | BF0   | 0.27848(73)   | -15.35429(12) | -15.37792(09) | -0.00036 | 0.02382 |
|       | BF1   | 0.13232(37)   | -15.37342(06) | -15.38282(03) | -0.00036 | 0.02413 |
|       | BF2   | 0.08441(22)   | -15.37923(05) | -15.38435(02) | -0.00036 | 0.02414 |
|       | BF3   | 0.06808(16)   | -15.38081(05) | -15.38484(02) | -0.00036 | 0.02441 |
|       | BF4   | 0.06179(20)   | -15.38135(04) | -15.38499(02) | -0.00036 | 0.02468 |
|       | ext full |           | -15.38877(44) | -15.38706(10) |            |               |
|       | ext w/o PW |         | -15.38758(52) | -15.38679(09) |            |               |
| 1.00  | PW    | 0.67302(100)  | -15.29788(10) | -15.36486(22) | -0.00032 | 0.02543 |
|       | BF0   | 0.24224(67)   | -15.35647(10) | -15.37570(08) | -0.00032 | 0.02382 |
|       | BF1   | 0.11261(29)   | -15.37226(07) | -15.37986(05) | -0.00032 | 0.02413 |
|       | BF2   | 0.07619(22)   | -15.37678(05) | -15.38098(04) | -0.00032 | 0.02414 |
|       | BF3   | 0.06177(20)   | -15.37821(03) | -15.38141(02) | -0.00032 | 0.02441 |
|       | BF4   | 0.05502(14)   | -15.37866(04) | -15.38163(03) | -0.00032 | 0.02468 |
|       | ext full |           | -15.38499(35) | -15.38347(06) |            |               |
|       | ext w/o PW |         | -15.38435(81) | -15.38325(03) |            |               |

TABLE II. Same as Table I for $r_s = 100$
| ζ    | Ψ    | \(\sigma^2/\sigma_0^2\) | VMC          | DMC          | \(\Delta T_0\) | \(\Delta FSE\) |
|------|------|----------------|--------------|--------------|----------------|----------------|
| 0.00 | PW   | 1.0000(30)    | -12.87447(19)| -12.95868(20)| -0.00036       | 0.01930        |
|      | BF0  | 0.3557(10)    | -12.94860(12)| -12.97655(07)| -0.00036       | 0.01803        |
|      | BF1  | 0.1728(04)    | -12.97104(05)| -12.98269(08)| -0.00036       | 0.01883        |
|      | BF2  | 0.1026(03)    | -12.97875(04)| -12.98476(03)| -0.00036       | 0.01876        |
|      | BF3  | 0.0804(02)    | -12.98078(04)| -12.98557(03)| -0.00036       | 0.01886        |
|      | BF4  | 0.0716(02)    | -12.98137(02)| -12.98572(02)| -0.00036       | 0.01893        |
|      | ext full |         | -12.98943(65)| -12.98819(12)|               |                |
|      | ext w/o PW |     | -12.98782(59)| -12.98786(27)|               |                |
| 0.42 | PW   | 0.96287(299)  | -12.88101(24)| -12.96112(18)| -0.00018       | 0.01930        |
|      | BF0  | 0.33762(89)   | -12.95121(10)| -12.97750(06)| -0.00018       | 0.01803        |
|      | BF1  | 0.16520(45)   | -12.97204(06)| -12.98279(03)| -0.00018       | 0.01883        |
|      | BF2  | 0.09097(26)   | -12.97913(04)| -12.98477(03)| -0.00018       | 0.01876        |
|      | BF3  | 0.07704(19)   | -12.98108(04)| -12.98537(03)| -0.00018       | 0.01886        |
|      | BF4  | 0.06876(19)   | -12.98179(03)| -12.98564(03)| -0.00018       | 0.01893        |
|      | ext full |         | -12.98943(57)| -12.98780(07)|               |                |
|      | ext w/o PW |     | -12.98777(37)| -12.98760(05)|               |                |
| 0.61 | PW   | 0.91729(294)  | -12.88814(19)| -12.96447(21)| -0.00022       | 0.01930        |
|      | BF0  | 0.32041(99)   | -12.95415(10)| -12.97834(06)| -0.00022       | 0.01803        |
|      | BF1  | 0.15444(40)   | -12.97320(05)| -12.98313(04)| -0.00022       | 0.01883        |
|      | BF2  | 0.09523(23)   | -12.97663(05)| -12.98488(03)| -0.00022       | 0.01876        |
|      | BF3  | 0.07506(18)   | -12.98150(04)| -12.98546(02)| -0.00022       | 0.01886        |
|      | BF4  | 0.06584(20)   | -12.98211(04)| -12.98562(02)| -0.00022       | 0.01893        |
|      | ext full |         | -12.98939(48)| -12.98768(09)|               |                |
|      | ext w/o PW |     | -12.98822(63)| -12.98748(17)|               |                |
| 0.79 | PW   | 0.83963(256)  | -12.89765(20)| -12.96749(13)| -0.00025       | 0.01930        |
|      | BF0  | 0.29635(74)   | -12.95744(10)| -12.97902(11)| -0.00025       | 0.01803        |
|      | BF1  | 0.14659(39)   | -12.97407(07)| -12.98321(03)| -0.00025       | 0.01883        |
|      | BF2  | 0.09018(23)   | -12.97979(04)| -12.98461(03)| -0.00025       | 0.01876        |
|      | BF3  | 0.07189(18)   | -12.98147(03)| -12.98508(02)| -0.00025       | 0.01886        |
|      | BF4  | 0.06351(18)   | -12.98203(04)| -12.98522(02)| -0.00025       | 0.01893        |
|      | ext full |         | -12.98867(39)| -12.98689(11)|               |                |
|      | ext w/o PW |     | -12.98751(44)| -12.98663(08)|               |                |
| 1.00 | PW   | 0.71979(221)  | -12.91080(17)| -12.96998(18)| -0.00022       | 0.01930        |
|      | BF0  | 0.26296(59)   | -12.96006(09)| -12.97809(05)| -0.00022       | 0.01803        |
|      | BF1  | 0.12702(33)   | -12.97426(05)| -12.98178(04)| -0.00022       | 0.01883        |
|      | BF2  | 0.08318(39)   | -12.97981(05)| -12.98289(02)| -0.00022       | 0.01876        |
|      | BF3  | 0.06682(18)   | -12.98021(04)| -12.98324(02)| -0.00022       | 0.01886        |
|      | BF4  | 0.06109(35)   | -12.98067(03)| -12.98338(02)| -0.00022       | 0.01893        |
|      | ext full |         | -12.98687(25)| -12.98516(12)|               |                |
|      | ext w/o PW |     | -12.98632(53)| -12.98470(07)|               |                |

**TABLE III.** Same as Table II for \(r_s = 120\)