Genetic algorithm for the pair distribution function of the electron gas

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Abstract

The pair distribution function of the electron gas is calculated using a parameterized generalization of quantum hypernetted chain approximation with the parameters being obtained by optimizing the system energy with a genetic algorithm. The functions so obtained are compared with Monte Carlo simulations performed by other authors in its variational and diffusion versions showing a very good agreement especially with the diffusion Monte Carlo results.

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I. INTRODUCTION

The Sommerfeld electron gas model[1] has proved to be very useful in describing many of the electronic properties of metallic solids. It represents the conduction electrons as a zero temperature ensemble of point charged fermions moving against a continuous neutralizing background that plays the role of the ionic lattice. In the simplest version of the model, fermions are considered spinless and the background is just characterized by a dielectric constant. If we have N fermions of mass m each one carrying a charge e, then the system Hamiltonian reads

$$H = \left(\frac{\hbar^2}{2m}\right)\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v\left(r_{ij}\right). \tag{1}$$

Here $v\left(r_{ij}\right)$ is the pair potential given by

$$v\left(r_{ij}\right) = \frac{e^2}{\varepsilon r_{ij}}, \tag{2}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ with $\mathbf{r}_i$ the position of the ith-particle and ε denoting the dielectric constant.

The equilibrium behavior of this system has been widely studied through quantal Monte Carlo simulations[2],[3] and also from a variety of many-body theories[4]-[8]. Many of them center on the pair distribution functions (PDF)[9]. If the we denote $\psi\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots,\mathbf{r}_N\right)$ the N-body wave function then the pair distribution function is given

$$\begin{aligned}\rho\left(\mathbf{r}_1\,,\mathbf{r}_2\right) &= \rho\left(\mathbf{r}_1\right)\rho\left(\mathbf{r}_2\right)g\left(\mathbf{r}_1\,,\mathbf{r}_2\right) \\ &= N\left(N-1\right)\frac{\int\cdots\int d\mathbf{r}_3\,d\mathbf{r}_4\,\cdots d\mathbf{r}_N\;\left|\psi\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots,\mathbf{r}_N\right)\right|^2}{\int\cdots\int d\mathbf{r}_1\,d\mathbf{r}_2\,\cdots d\mathbf{r}_N\;\left|\psi\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots,\mathbf{r}_N\right)\right|^2}\end{aligned} \tag{3}$$

where the integrations are over the whole volume and

$$\rho\left(\mathbf{r}_1\right) = N\frac{\int\cdots\int d\mathbf{r}_2\,d\mathbf{r}_3\,\cdots d\mathbf{r}_N\;\left|\psi\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots,\mathbf{r}_N\right)\right|^2}{\int\cdots\int d\mathbf{r}_1\,d\mathbf{r}_2\,\cdots d\mathbf{r}_N\;\left|\psi\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots,\mathbf{r}_N\right)\right|^2} \tag{4}$$

is the one point distribution function. The function $g\left(\mathbf{r}_1\,,\mathbf{r}_2\right)$ is the pair correlation function (PCF). For homogenous systems (as will be considered here) $\rho\left(\mathbf{r}_i\right)$ gives the electrons

number density $\rho(\mathbf{r}_i) = \rho = N/V$ (V = system volume) and the PDF and PCF depend only on the particles separation: $\rho(r_{12}) = \rho^2 g(r_{12})$.

For the homogeneous electron gas in three and lower dimensions, the PDF as well its Fourier transform, the static structure factor $S(k)$, have been studied by several authors using diverse analytical techniques[6] and also simulations methods. In 3D, we mention random phase approximation (RPA) calculations[10], diagrammatic ladder approximations[11], the local-field based method of Singwi, Tosi, Land and Sjölander (STLS)[12], calculations with quantum hypernetted chain equations (QHNC)[13] and also techniques that use parameterized PDF, the parameters being determined from known independent theoretical or simulation results[14]-[17]. From the side of Monte Carlo quantum simulations in both -the variational and diffusion- versions, the work by Ortiz and Ballone[18] extends in several ways previous results of Ceperley and Alder[2],[3].

Most of these approaches lean on the variational principle according to which the energy of the ground state E_0 is a lower bound for the Hamiltonian mean value as calculated using any trial wave function $\psi_T(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$:

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \geq E_0. \tag{5}$$

As trial function a factorized form

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = F(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)\, \psi_0(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \tag{6}$$

is frequently used. Here $\psi_0(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ denotes the system wave function when the interactions are turned off ($v(r_{ij}) \equiv 0$). It is an antisymmetric function under particles permutations. We can write

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = \sum_P (-1)^P P\{\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \cdots, \phi_N(\mathbf{r}_N)\} = \det[\phi_{\alpha_i}(\mathbf{r}_j)] \tag{7}$$

where P is the permutation operator that interchanges the particle positions, $\phi_{\alpha_i}(\mathbf{r}_j)$ is the wave function of an isolated particle and $\det[\phi_{\alpha_i}(\mathbf{r}_j)]$ means the Slater determinant. The symmetric factor $F(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ accounts for the correlations among the particles when the interactions are turned on. The N-body correlation factor can be factorized according

to Jastrow[19]:

$$F\left(\mathbf{r}_1\,,\mathbf{r}_2\,,\cdots\,,\mathbf{r}_N\,\right)=\prod_{i<j}f\left(\mathbf{r}_i\,,\mathbf{r}_j\,\right). \tag{8}$$

In this work we consider the evaluation of the PDF for the homogeneous 3D electron gas starting from a parameterized trial wave function of the form given by Eqs. (6-8) with the parameters obtained by optimizing the system energy by means of a genetic algorithm.

Genetic algorithms[20]-[21] form part, together with evolutionary programming[22],[23], game-playing strategies[24], genetic programming[25] and other related techniques, of a relatively new class of optimization algorithms which are based on the Darwinian evolution principle[26]. In particular, genetic algorithms tackle even complex problems with surprising efficiency and robustness. In Physics they have been used in calculations that involve from simple quantum systems[27] to astrophysical systems[28], running through lattice models for spin glasses[29], molecules[30] and clusters[31]. More recently[32] we have developed a genetic algorithm for the PDF of the one-dimensional electron gas in what, at our knowledge, is the first application of this kind of algorithm to describe many-body systems in the thermodynamic limit..

In general, a genetic algorithm is based on three main statements:

a) It is a process that works at the chromosomic level. Each individual is codified as a set of chromosomes.

b) The process follows the Darwinian theory of evolution, say, the survival and reproduction of those individuals that best adapt in a changing environment.

c) The evolutionary process takes place at the reproduction stage. It is in this stage when mutation and crossover occurs. As a result, the progeny chromosomes can differ from their parents ones.

Starting from a guess initial population, a genetic algorithm basically generates consecutive generations (offprints). These are formed by a set of chromosomes, or character (genes) chains, which represent possible solutions to the problem under consideration. At each algorithm step, a fitness function is applied to the whole set of chromosomes of the corresponding generation in order to check the goodness of the codified solution. Then, according to their fitting capacity, couples of chromosomes, to which the crossover operator will be applied, are chosen. Also, at each step, a mutation operator is applied to a number of randomly chosen chromosomes.

The two most commonly used methods to randomly select the chromosomes are:

i) *The roulette wheel algorithm.* It consists in building a roulette, so that to each chromosome corresponds a circular sector proportional to its fitness.

ii) *The tournament method.* After shuffling the population, their chromosomes are made to compete among them in groups of a given size (generally in pairs). The winners will be those chromosomes with highest fitness. If we consider a binary tournament, say the competition is between pairs, the population must be shuffled twice. This technique guarantees copies of the best individual among the parents of the next generation.

After this selection, we proceed with the sexual reproduction or crossing of the chosen individuals. In this stage, the survivors exchange chromosomic material and the resulting chromosomes will codify the individuals of the next generation. The forms of sexual reproduction most commonly used are:

i) With one crossing point. This point is randomly chosen on the chain length, and all the chain portion between the crossing point and the chain end is exchanged.

ii) With two crossing points. The portion to be exchanged is in between two randomly chosen points.

For the algorithm implementation, the crossover normally has an assigned percentage that determines the frequency of its occurrence. This means that not all of the chromosomes will exchange material but some of them will pass intact to the next generation. As a matter of fact, there is a technique, named elitism, in which the fittest individual along several generations does not cross with any of the other ones and keeps intact until an individual fitter than itself appears.

Besides the selection and crossover, there is another operation, mutation, that produces a change in one of the characters or genes of a randomly chosen chromosome. This operation allows to introduce new chromosomic material into the population. As for the crossover, the mutation is handled as a percentage that determines its occurrence frequency. This percentage is, generally, not greater than 5%, quite below the crossover percentage.

Once the selected chromosomes have been crossed and muted, we need some substitution method. Namely, we must choose, among those individuals, which ones will be substituted for the new progeny. Two main substitution ways are usually considered. In one of them, all modified parents are substituted for the generated new individuals. In this way an individual does never coexist with its parents. In the other one, only the worse fitted individuals of the

whole population are substituted, thus allowing the coexistence among parents and progeny.

Since the answer to our problem is almost always unknown, we must establish some criterion to stop the algorithm. We can mention two such criteria: i) the algorithm is run along a maximum number of generations; ii) the algorithm is ended when the population stabilization has been reached, i.e. when all, or most of, the individuals have the same fitness.

In Section III we will apply these ideas to determine the parameters appearing in the expression for the 3D electron gas PDF that we propose in Section II.

II. PARAMETERIZED PDF

We assume that the trial wave function for the system of N-spinless electrons with Hamiltonian given by Eqs.(1,2) has the form of Eq.(6) where we use for the ideal part $\psi_0(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ a parameterized generalization of an expression given by Lado[33] and for the Jastrow correlation factor also a parameterized expression containing a random phase approximation (RPA) pseudopotential[2],[34]. Specifically we propose

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = \exp\left\{\frac{1}{2}\sum_{i<j}\left[\alpha w_0(r_{ij}) - \beta u_{RPA}(r_{ij})\right]\right\} \tag{9}$$

where α and β are the parameters to adjust.

In Eq.(9) the ideal gas effective potential $w_0(r)$ is defined

$$w_0(r) = \ln g_0(r) - \frac{1}{(2\pi)^3 \rho}\int d\mathbf{k} e^{-i\mathbf{k}.\mathbf{r}} \frac{[S_0(k) - 1]^2}{S_0(k)}. \tag{10}$$

Here $g_0(r)$ and $S_0(k)$ are the ideal PCF and structure factor, respectively, whose expressions are[35],[36]:

$$g_0(r) = 1 - \frac{9}{2}\left[\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}\right]^2 \tag{11}$$

and

$$S_0(k) = \begin{cases} 1 & k > 2k_F \\ \frac{3}{4}\frac{k}{k_F} - \frac{1}{16}\left(\frac{k}{k_F}\right)^3 & k < 2k_F \end{cases} \tag{12}$$

with k_F the Fermi momentum $k_F = (3\pi^2\rho^*)^{\frac{1}{3}}$ where $\rho^* = \rho a_0$ (a_0 is the Bohr radius).

The RPA pseudopotential, on the other hand, reads

$$2\rho^{*}u_{RPA}\left(k\right)=-\frac{1}{S_{0}\left(k\right)}+\left[\frac{1}{S_{0}\left(k\right)^{2}}+\frac{4m\rho^{*}\widetilde{v}\left(k\right)}{\hbar^{2}k^{2}}\right]^{1/2} \tag{13}$$

where $\widetilde{v}\left(k\right)$ is the Fourier transform of the interparticle potential $v\left(r\right)$.

It is worth mentioning that in the genetic algorithm me have develop for the 1D electron gas in Ref.[32], instead of using the RPA pseudopotential in Eq.(9) we assume that $u\left(r\right)$ is an unknown function and the algorithm is designed to completely obtain it. Here, a parameterized form for the pseudopotential is proposed *a priori* and the algorithm looks for the optimal parameters.

In principle, to calculate PDF from Eq.(3) we have to integrate the square of the wave function over $3N$ coordinates. To avoid this formidable task use is done of a modified form of the hypernetted chain approximation (HNC) for which the PDF is written as a single integral equation involving just a pair of particles. We write, ignoring all the elemental diagrams[37],

$$g\left(r\right)=\exp\left[\alpha w_{0}\left(r\right)-\beta u_{RPA}\left(r\right)+N\left(r\right)\right] \tag{14}$$

$$N\left(r\right)=\rho\int\left[g\left(r'\right)-1-N\left(r'\right)\right]\left[g\left(\left|\mathbf{r}-\mathbf{r}'\right|\right)-1\right]d\mathbf{r} \tag{15}$$

where $N\left(r\right)$ denotes the sum of nodal diagrams. Eq. (14) without the term with α in the exponential has the form of the PCF for a system of bosons (see v.g. Eq.(40) in Ref. [37] where the nodal diagrams are denoted D and the elementals diagrams E must be taken zero). The term with α adds the ideal part that contains the proper symmetry for fermions.

Finally, in the variational approach which is implicit in Eq.(5), we need an expression for the Hamiltonian mean value. Making use of Jackson-Feenberg identity[38] we obtain

$$\frac{E}{N}=\frac{\rho}{2}\int d\mathbf{r}g\left(r\right)\left[-\frac{\hbar^{2}}{4m}\nabla^{2}\ln f^{2}\left(r\right)+v\left(r\right)\right]. \tag{16}$$

III. PARAMETERS OPTIMIZATION

Our problem is to solve for $g\left(r\right)$ the integral equation given by Eqs.(14 and 15) with the parameters α and β determined by demanding that the energy functional $E=E\left\{g\left(r\right)\right\}$

given by Eq.(16) be minimum. To this end we use a genetic algorithm.

We proceed by first generating the initial population, which is formed by N_p random replicas of the two numbers string (that represents one population individual) $\gamma^{(\alpha)}, \gamma^{(\beta)}$ where $\gamma^{(\alpha)} \in [0,1]$ is a random real number (rounded to an established number n of decimals) which is assigned to the parameter α. Given a string $\gamma^{(\alpha)}, \gamma^{(\beta)}$, the *encoding* consists in replacing the sequence of real numbers by a single natural number obtained by putting their decimals parts one next to the other. Thus if $\gamma^{(\alpha)} = 0.\gamma_1^{(\alpha)}\ \gamma_2^{(\alpha)}...\gamma_n^{(\alpha)}$ and $\gamma^{(\beta)} = 0.\gamma_1^{(\beta)}\ \gamma_2^{(\beta)}...\gamma_n^{(\beta)}$ then we have the chain :

$$\gamma_1^{(\alpha)}\gamma_2^{(\alpha)}...\gamma_n^{(\alpha)}\gamma_1^{(\beta)}\gamma_2^{(\beta)}...\gamma_n^{(\beta)}$$

and the population is the set

$$\left\{\left(\gamma_1^{(\alpha)}\gamma_2^{(\alpha)}...\gamma_n^{(\alpha)}\gamma_1^{(\beta)}\gamma_2^{(\beta)}...\gamma_n^{(\beta)}\right)_r \qquad r = 1, 2, \cdots, N_p\right\}$$

In genetic terms, the encoding produces the chromosomic structure of the individuals (replica string). The inverse process is called *decoding* and returns the parameters α and β corresponding to each individual. In the decoding we allow the returned parameters be multiplied by a constant factor $\eta > 1$ in order that the parameters can take values in an interval wider than $[0,1]$. We define the fitness of the rth individual as $f_r = e^{-E_r}$ where E_r is the energy calculated using Eq.(16) when $g(r)$ is calculated from Eqs.(14 and 15) for the parameters α and β obtained by decoding the chromosome structure of the rth individual of the population. A solution is reached when $f_r \approx 1$ for some individual r in some of the successive populations obtained in the evolution process.

The calculation proceeds by dividing the population of N_p replicas into $N_p/2$ couples. The couples are randomly chosen by using the roulette wheel algorithm[20]. This is done by defining the sums $F = \sum_{r=1}^{N_p} f_r$ and $S_\delta = \sum_{r=1}^{\delta} f_r \ \ (\delta = 1, 2, ..., N_p)$. Then, a random number $\kappa \in [0, F]$ is generated and the unique index δ such that $S_{\delta-1} \leq \kappa \leq S_\delta$ is picked up.

Once the first generation of replicas (parents) has been generated and divided into couples, the second generation (offspring) can be generated by applying the crossover operator between the members of each one. At times , some of the members of the new replicas generation can be changed by applying the mutation operator.

TABLE I: Parameters α and β

r_s	α	β
1	2.2227	1.6456
2	7.8707	14.865
3	9.6789	30.526
6	14.710	43.030
10	44.974	18.464
50	-6834.17	128.71

Given a couple of replicas, the crossover operator is defined by generating a new random number $c \in [0, 1]$ which is compared with a pre-established crossover probability $p \in [0, 1]$. If $c \leq p$, the crossover operator acts by interchanging all the digits from the sth position to the end of the replica between the members of the couple. Here s is a random integer such that $1 \leq s \leq 2n$. for example if the couple is

153280472...337

768325399...069

and $s = 4$, the new offspring couple will be

153225399...069

768380472...337.

To apply the mutation operator we first randomly select those offsprings that will mutate. Then, for each of these offsprings, a gene (a digit) randomly chosen is changed by a random integer number $\ell \in [0, 9]$ .The algorithm is stopped when a solution is reached for the parameters α and β.

IV. RESULTS

As it is easily seen, the electron gas is completely determined by giving just its density ρ or, as it is custom in many-body theory, the Wigner-Seitz radius r_s defined $r_s = [3/4\pi\rho]^{1/3}$. Here we have applied the procedure described above, to an electron gas at metallic densities: $1 \leq r_s \leq 10$ and also at $r_s = 50$. We use in our calculations $N_p = 150$ and $n = 5$. The factor η, in turn, is moved in each case to give reasonable values for the parameters α and β. In Table I we show the parameters α and β obtained for the diverse values of r_s considered.

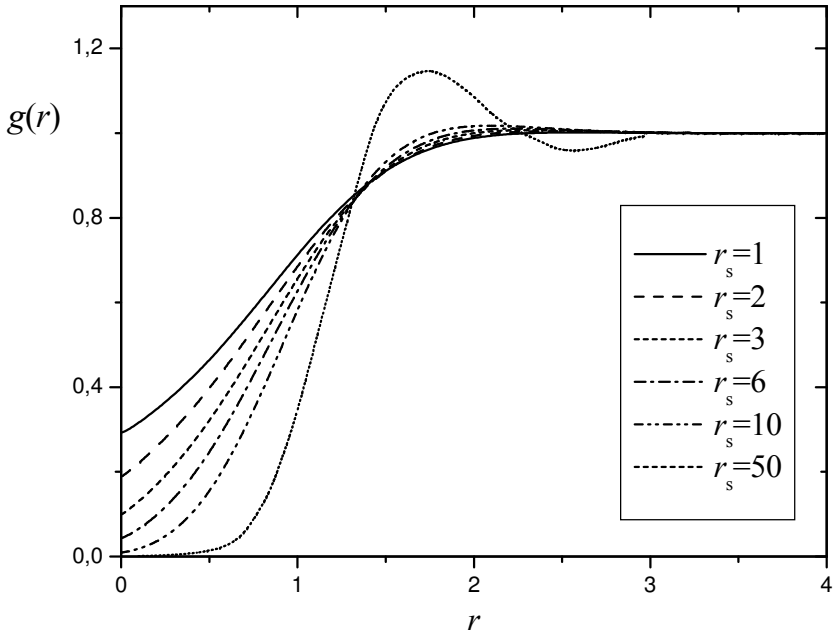

FIG. 1: The functions $g\,(r)$ for the homogenous electron gas at r_s=1,2,3,6,10 and 50 obtained in this work.

Note the change in the parameters tendency at $r_s = 50$. By the way, we were unable to reach convergence for values of r_s greater than this one.

Figs. 1 to 3 show the corresponding $g\,(r)'$s. In Fig. 1 we put all together the curves we have obtained . We observe the characteristic features of the electron gas: when the density increases (r_s decreases) the behavior tends to that of an ideal paramagnetic gas of fermions with contact value 1/2 and rapidly going to the asymptotic value 1. When the density decreases the correlation functions become more structured showing, in particular, a more pronounced Coulomb hole near contact.

In Figs. 2 and 3 comparison is done of our results with those obtained from variational as well as diffusion Monte Carlo simulations performed by other authors[18],[13],[39]. A first remark is the existing differences between variational and diffusion results particularly for low values of r_s. Also must be noticed the good agreement of the results of this work with those obtained from diffusion Monte Carlo calculations.

It is worth mentioning that the time to obtain one of our curves by running the complete algorithm with a Pentium IV is tipically of the order of 50 hours for the metallic densities.

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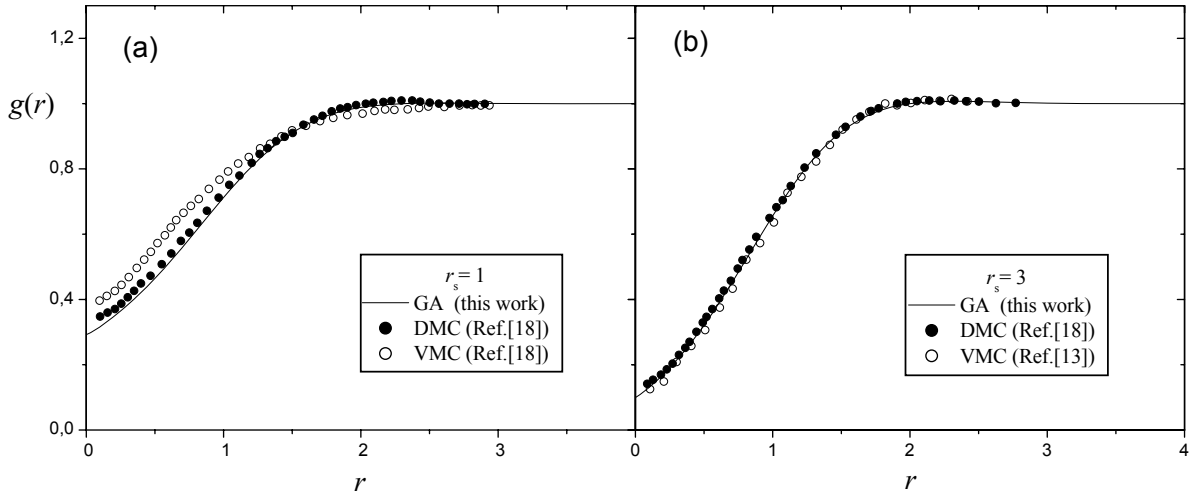

FIG. 2: The functions $g(r)$ for the homogenous electron obtained in this work compared with variational and diffusion Monte Carlo results. (a): r_s=1; (b): r_s=3.

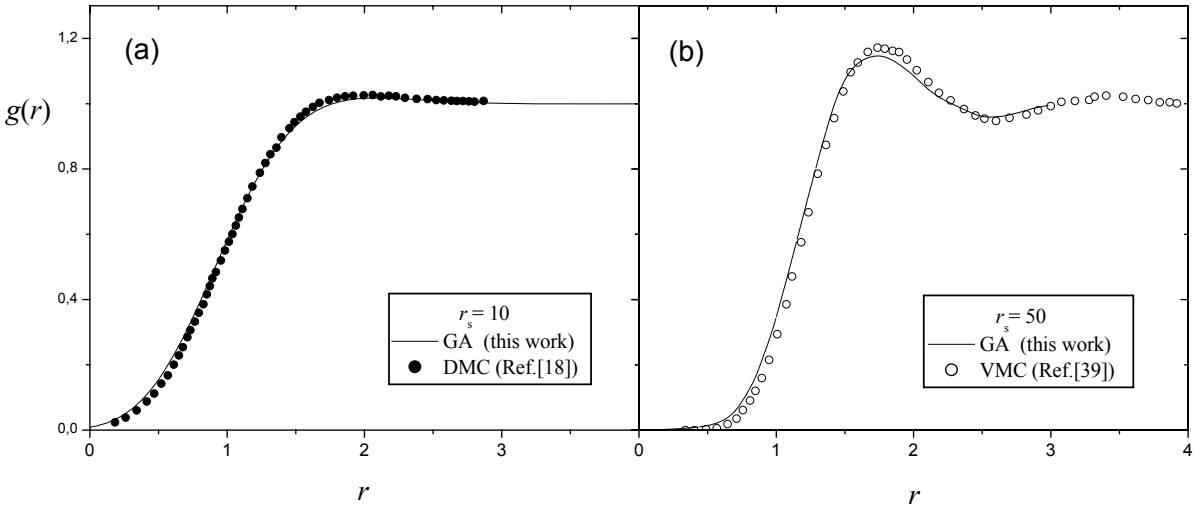

FIG. 3: The functions $g(r)$ for the homogenous electron obtained in this work compared with variational and diffusion Monte Carlo results. (a): r_s=10; (b): r_s=50.

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[1] L. Hoddeson, G. Baym and M. Eckert, Rev. Mod. Phys. **59**, 287 (1987).

[2] D.M. Ceperley, Phys. Rev. B **18**, 3126 (1978).

[3] D.M. Ceperley and B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980).

[4] N.H. March, W.H. Young and S. Sampanthar, *The Many-Body Problem in Quantum Mechanics* (Cambridge University Press, London, 1967).

[5] A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw Hill, New York, 1981).

[6] G.D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).

[7] N.H. March and M.P. Tosi, *Coulomb Liquids* (Academic, London, 1984).

[8] W.D. Kraeft, D. Kremp, W. Ebeling and G. Ropke, *Quantum Statistics of Charged Particle Systems* (Plenum, New York, 1986).

[9] K.S. Singwi and M.P. Tosi, Solid State Phys., **36**, 177 (1981).

[10] D. Pines and P. Nozieres, *Theory of Quantum Liquids* (Benjamin, New York, 1966).

[11] H. Yasuhara, Solid State Commun., **11**, 1481 (1972); J. Phys. Soc. Jpn., **36**, 361 (1974); Physica, **78**, 420 (1974).

[12] K.S. Singwi, M.P. Tosi, R.H. Land and A. Sjölander, Phys. Rev., **176**, 589 (1968).

[13] L.J. Lantto, Phys. Rev. B, **22**, 1380 (1980).

[14] A.K. Rajagopal, J.C. Kimball and M. Banarjee, Phys. Rev. B., **18**, 2339 (1978).

[15] V. Contini, G. Mazzone and F. Sacchetti, Phys. Rev. B., **33**, 712 (1986).

[16] F. Vericat, G. Pastore and M.P. Tosi, Nuovo Cimento D, **8**, 59 (1986).

[17] P. Gori-Giorgi and J.P. Perdew, Phys. Rev. B., **66**,165118 (2002).

[18] G. Ortiz and P. Ballone, Phys. Rev. B, **50**, 1391 (1994); erratum: Phys. Rev. B., **56**, 9970 (1997).

[19] R.J. Jastrow, Phys. Rev., **98**, 1479 (1955).

[20] D.E. Goldberg, *Genetic Algorithm in Search, Optimization and Machine Learning* (Addison-Wesley, Reading, MA, 1989).

[21] M. Mitchell, *An Introduction to Genetic Algorithm* (Prentice Hall, 1998).

[22] D. Fogel, *Evolutionary Computation* (IEEE Press, 1996).

[23] T. Bäck, *Evolutionary Algorithm in Theory and Practice* (Oxford Press, 1996).

[24] *Genetic Algorithms and Simulated Annealing*, edited by L. Davis (Pitman. London. 1987)-

[25] J.R. Koza, *Genetic Programming: On the Programming of Computers by Means of Natural Selection* (MIT, Cambridge, MA,1992).

[26] J.H. Holland, *Adaptation in Natural and Artificial Systems* (University of Michigan, Ann

Arbor, MI, 1975).

[27] I. Grogorenko and M.E. García, Physica A, **291**, 439 (2001); **313**, 463 (2002).

[28] P. Charbonneau, The Astrophysical Journal, Supplement Series, **101**, 309 (1995).

[29] A. Prügel-Bennet and J.L. Shapiro, Physica D, **104**, 75 (1997).

[30] M.A. Moret, P.G. Pascutti, P.M. Bisand and K.C. Mundin, Physica A, **363**, 260 (2006).

[31] Y. Zeiri, Comp. Phys. Comm., **103**, 28 (1997).

[32] C.O. Stoico, D.G. Renzi and F. Vericat,.Physica A, **387**, 159 (2008).

[33] F. Lado, J. Chem. Phys. **47**, 5369 (1967).

[34] T. Gaskell, Proc. Phys. Soc. **77**, 1182 (1961); **80**, 1091 (1962).

[35] G. Placzek, in *Proceedings of the Second Berkeley Symposium on Mathematical statistics and Probability* (University of California Press, Berkeley, California, 1951).

[36] F. London, J. Chem. Phys., **11**, 203 (1943).

[37] C.O. Stoico, C.M. Carlevaro, D.G. Renzi and F. Vericat, Physica E, **42**, 1691 (2010).

[38] Feenberg, *Theory of Quantum Fluids* (Academic Press, New York, 1969).

[39] D.M. Ceperley and B.J. Alder, Journal de Physique, **41**, C7-295 (1980).