

# An inhomogeneous and anisotropic Jastrow function for non-uniform many-electron systems

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## Abstract

Quantum Monte Carlo simulations of interacting electrons in solids often use Slater–Jastrow trial wave functions. The Jastrow function takes into account correlations between pairs of electrons. In simulations of solids, it is common to use a Jastrow function which is both homogeneous and isotropic. The use of a homogeneous and isotropic Jastrow factor is questionable in applications to systems with strong density inhomogeneities, such as surfaces and multilayers. By generalizing the original derivation of the RPA Jastrow factor for the homogeneous electron gas (HEG) [Proc. Phys. Soc. 77 (1961) 1182; 80 (1962) 1091] to inhomogeneous systems we derive a scheme for generating inhomogeneous and anisotropic Jastrow factors for use in non-uniform systems, from the non-interacting static structure factor and density of the system. We discuss aspects of our scheme and illustrate it with a first application to an inhomogeneous electron gas. © 2001 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

In this paper, we consider Slater–Jastrow trial wave function,  $\Psi = De^J$ , where  $D$  is a Slater determinant and  $J$  the Jastrow factor that takes account of the electronic correlations. Such wave functions are employed in variational quantum Monte Carlo (VQMC) simulations of solids [3,4], where an approximate many-electron ground state is obtained by numerically optimizing an explicit parametrized trial wave function. Remarkably better results are obtained from VQMC calculations using Slater–Jastrow functions than from Hartree–Fock (HF) or density-functional theory within the local density approximation (LDA). For example, cohesive energies obtained using VQMC are typically an order of magnitude more accurate than those obtained employing HF or LDA [5–9].

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We use a Slater determinant of LDA orbitals and a Jastrow factor that includes pairwise correlation terms  $u(\mathbf{r}_i, \mathbf{r}_j)$ . In simulation of solids  $u$  is usually taken to be both homogeneous and isotropic, i.e.,  $u(\mathbf{r}_i, \mathbf{r}_j)$  is assumed to depend only on the inter-electronic distance  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ .

The long-range behaviour of  $u(\mathbf{r}_i, \mathbf{r}_j)$  is determined by the zero-point motion of the plasmons, both in homogeneous [10,11] and inhomogeneous systems [12] while the short-range behaviour is governed by the so-called cusp condition [13,14]. Gaskell minimized the variational energy of the uniform electron gas in the random-phase approximation and found a Jastrow function which combined both the short-range and the long-range behaviour. Ceperley used this Jastrow function in his variational Monte Carlo calculations of the spin-unpolarized homogeneous electron gas (HEG) [15].

Here we generalize Gaskell's approach to inhomogeneous systems and derive an inhomogeneous and anisotropic Jastrow factor that depends on the non-interacting structure factor and density of the system. The Jastrow factor is represented as a double Fourier integral. The full interacting many-electron Hamiltonian  $\hat{H}$  is expressed as a function of the plane-wave expansion coefficients of the Jastrow function and, within the random-phase approximation (RPA)  $\hat{H}$  is minimized with respect to these coefficients. This way the approximated ground state energy is obtained, and the trial wavefunction of the system can be constructed from the resulting inhomogeneous and anisotropic Jastrow function. In the homogeneous limit, our approach reduces to that of Gaskell.

The rest of the paper is organized as follows. In Section 2.1, we describe the formalism used in Gaskell's original derivation of the Jastrow function for the HEG. Section 2.2 presents our generalization to systems with density inhomogeneities where, for the sake of simplicity, we consider systems with density variations in only one direction. Section 3 discusses the numerical results obtained for the IHEG, and Section 4 concludes.

## 2. Formalism

A Slater–Jastrow trial wave function is the product of a totally antisymmetric Slater determinant  $D$  and a totally symmetric Jastrow factor  $e^J$ :  $\Psi = De^J$ . The orbitals used in  $D$  are obtained from LDA calculations. Here we consider spin-unpolarized systems. The Slater determinant builds in exchange effects but neglects the electronic correlations caused by the Coulomb interactions. The most important correlation effects occur when pairs of electrons approach each other, and these may be included by choosing pairwise Jastrow factors of the form

$$J = - \sum_{i,j} u(\mathbf{r}_i, \mathbf{r}_j), \quad (1)$$

where  $u(\mathbf{r}_i, \mathbf{r}_j) = u(\mathbf{r}_j, \mathbf{r}_i)$ . So the trial wave function can be written as

$$\Psi(\mathbf{R}) = D \exp \left[ - \sum_{i,j} u(\mathbf{r}_i, \mathbf{r}_j) \right]. \quad (2)$$

Note that we include the  $i = j$  terms in the sum over  $i$  and  $j$ , which are omitted by many authors as they give a constant contribution for the HEG. (Unless otherwise is stated, we use atomic units throughout, i.e.,  $e^2 = \hbar = m_e = 1$ .)

The full interacting many-electron Hamiltonian is given by

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \hat{V}_{ext}, \quad (3)$$

where  $\hat{T}$  and  $\hat{V}_{ee}$  are the kinetic energy and the electron–electron interaction operators, respectively and  $\hat{V}_{ext}$  is an external potential. The expectation value of the energy with respect to the above trial wave function can be written as (the normalized  $\Psi$  is taken)

$$E = \langle \Psi | H | \Psi \rangle = \sum_{i=1}^N \epsilon_i + \int d\mathbf{r} n(\mathbf{r}) V_{\text{ext}}(\mathbf{r}) - \int d\mathbf{r} n(\mathbf{r}) V_s(\mathbf{r}) + \langle T_2 \rangle + \langle V_{\text{ee}} \rangle, \quad (4)$$

where  $V_s$  is the effective single-particle potential associated with the orbitals in the Slater determinant,  $\epsilon_i$  are the energy eigenvalues which correspond to such one electron orbitals and  $n(\mathbf{r})$  is the electron density.  $\langle T_2 \rangle$  and  $\langle V_{\text{ee}} \rangle$  are defined as

$$\langle T_2 \rangle = \int d\mathbf{R} \Psi^*(\mathbf{R}) \Psi(\mathbf{R}) \left[ \sum_{m=1}^N \nabla_m \left( \sum_{i,j} U(\mathbf{r}_i, \mathbf{r}_j) \right) \cdot \nabla_m \left( \sum_{i,j} U(\mathbf{r}_i, \mathbf{r}_j) \right) \right] \quad (5)$$

and

$$\langle V_{\text{ee}} \rangle = \int d\mathbf{R} \Psi^*(\mathbf{R}) \Psi(\mathbf{R}) \left( \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right). \quad (6)$$

Here  $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$  represents all electron coordinates. Several different types of Jastrow factors are commonly used, the best known are based on the RPA in the form due to Gaskell and the form based on the RPA of Bohm and Pines [10,11]. Here we will briefly describe the Jastrow factor due to Gaskell for the HEG before presenting its generalization to inhomogeneous systems.

### 2.1. The homogeneous RPA Jastrow factor

For homogeneous systems the correlation term  $u$  depends only on the inter-electronic distance  $r_{ij}$  and may be expressed as follows:

$$u(\mathbf{r}_i, \mathbf{r}_j) = u(r_{ij}) = \sum_k u(k) e^{ikr_{ij}}, \quad (7)$$

where  $k$  is the modulus of the total wavevector. Also, the single-particle orbitals are a set of planewaves. Inserting the above expression in Eq. (4), the total energy in the random-phase approximation of  $T_2$  can be written as [1,2]

$$E = \sum_{k \leq k_F} \frac{1}{2} k^2 + 2N^2 \sum_{\mathbf{k}} k^2 u^2(k) S(k) + 2\pi n_0 \sum_{\mathbf{k}} \frac{1}{k^2} [S(k) - 1], \quad (8)$$

where  $NS(k) = \langle \Psi | \hat{n}_{\mathbf{k}} \hat{n}_{\mathbf{k}}^* | \Psi \rangle$  is the static structure factor of the uniform interacting electron gas and  $\hat{n}_{\mathbf{k}} = \sum_i e^{i\mathbf{k} \cdot \mathbf{r}_i}$  are the number density operators.  $k_F$  and  $n_0 = N/V$  are the Fermi energy and the average electron density, respectively,  $N$  being the total number of electrons in the system and  $V$  the volume. Gaskell assumed that the structure factor for the interacting electron gas is close to that of the non-interacting electron gas and, for a small Jastrow function  $u(\mathbf{r})$ <sup>1</sup> can be approximated by the perturbation formula [1,2]

$$S(k) = \frac{S_0(k)}{1 + 4u(k)S_0(k)}, \quad (9)$$

where  $S_0(k)$  is the structure factor of the non-interacting electron gas [16]. The variational energy in the random-phase approximation (Eq. (3)) can then be minimized with respect to  $u(k)$  to yield

<sup>1</sup> This corresponds to the high density limit.

$$u(k) = \frac{-1}{4S_0(k)} + \frac{1}{4} \left[ \frac{1}{4(S_0(k))^2} + \frac{16\pi n_0}{k^4} \right]^{1/2}. \quad (10)$$

## 2.2. The inhomogeneous RPA Jastrow factor

Here we consider the case of an inhomogeneous system translationally invariant in the plane perpendicular to the  $z$ -axis. In this case  $u$  can be written as

$$u(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{q}} \sum_{k_{z_1}, k_{z_2}} u_{k_{z_1}, k_{z_2}} e^{i\mathbf{q} \cdot (\mathbf{r}_{\parallel 1} - \mathbf{r}_{\parallel 2})} e^{ik_{z_1} z_1} e^{ik_{z_2} z_2}, \quad (11)$$

where  $\mathbf{r} = (\mathbf{r}_{\parallel}, z)$  and  $\mathbf{k} = (\mathbf{q}, k_z) \cdot u_{k_{z_1}, k_{z_2}}$  are the two-dimensional Fourier coefficients of the correlation function  $u$

$$u_{k_{z_1}, k_{z_2}}(\mathbf{q}) = \frac{1}{V} \int d\mathbf{r}_{\parallel} e^{i\mathbf{q} \cdot \mathbf{r}_{\parallel}} \int dz_1 \int dz_2 e^{ik_{z_1} z_1} e^{-ik_{z_2} z_2} u(\mathbf{r}_{\parallel}, z_1, z_2). \quad (12)$$

We use the following definition of the number density operator:  $\hat{n}_{\mathbf{q}, k_z} = \sum_i e^{i\mathbf{q} \cdot \mathbf{r}_{\parallel i}} e^{ik_z z_i}$ , so that the Slater–Jastrow trial wave function is given by

$$\Psi = D \exp \left[ - \sum_{\mathbf{q}} \sum_{k_{z_1}, k_{z_2}} u_{k_{z_1}, k_{z_2}}(\mathbf{q}) \hat{n}_{\mathbf{q}, k_{z_1}} \hat{n}_{\mathbf{q}, k_{z_2}}^* \right]. \quad (13)$$

### 2.2.1. Deriving an approximation for the inhomogeneous structure factor

In this section, we develop an approximation based on the RPA to obtain the interacting structure factor in terms of Fourier coefficients of the above Jastrow factor. Let us define

$$\Psi(\lambda) = D \exp \left[ - \lambda \sum_{\mathbf{q}} \sum_{k_{z_1}, k_{z_2}} u_{k_{z_1}, k_{z_2}}(\mathbf{q}) \hat{n}_{\mathbf{q}, k_{z_1}} \hat{n}_{\mathbf{q}, k_{z_2}}^* \right]. \quad (14)$$

The expectation value we need to calculate is of the form

$$I(\lambda) \equiv \frac{\langle \Psi(\lambda) | \hat{n}_{\mathbf{q}, k_{z_1}} \hat{n}_{\mathbf{q}, k_{z_2}}^* | \Psi(\lambda) \rangle}{\langle \Psi(\lambda) | \Psi(\lambda) \rangle}. \quad (15)$$

with  $\lambda = 1$ . With the above trial function this becomes

$$I(\lambda) = \frac{\int DD^* \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_2, k_{z_2}}^* \exp \left[ - 2\lambda \sum_{\mathbf{q}_2} \sum_{k_{z_3}, k_{z_4}} u_{k_{z_3}, k_{z_4}}(\mathbf{q}_2) \hat{n}_{\mathbf{q}_2, k_{z_3}} \hat{n}_{\mathbf{q}_2, k_{z_4}}^* \right]}{\int DD^* \exp \left[ - 2\lambda \sum_{\mathbf{q}_2} \sum_{k_{z_3}, k_{z_4}} u_{k_{z_3}, k_{z_4}}(\mathbf{q}_2) \hat{n}_{\mathbf{q}_2, k_{z_3}} \hat{n}_{\mathbf{q}_2, k_{z_4}}^* \right]}. \quad (16)$$

Following Gaskell we use the identity

$$\frac{1}{I(\lambda)} - \frac{1}{I(0)} = \int_0^\lambda \frac{\partial}{\partial \lambda'} \left[ \frac{1}{I(\lambda')} \right] d\lambda' \quad (17)$$

to obtain a perturbative approximation for  $I(1)$ . Taking the derivative inside the integral with respect to  $\lambda$  and expanding in a Taylor series the leading term is

$$\begin{aligned}
\left. \frac{\partial}{\partial \lambda'} \left( \frac{1}{I(\lambda')} \right) \right|_{\lambda=0} &= 4u_{k_{z_1}, k_{z_2}}(\mathbf{q}_1) \left[ \frac{\langle 0 | (\hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^*)^2 | 0 \rangle - \langle 0 | \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle^2}{\langle 0 | \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle^2} \right] \\
&+ 2 \sum_{\mathbf{q}_1, k_{z_3}, k_{z_4} (\mathbf{q}_2 \neq \pm \mathbf{q}_1, k_{z_3} \neq k_{z_1}, k_{z_4} \neq k_{z_2})} u_{k_{z_3}, k_{z_4}}(\mathbf{q}_2) \\
&\times \left[ \frac{\langle 0 | \hat{n}_{\mathbf{q}_2, k_{z_3}} \hat{n}_{\mathbf{q}_2, k_{z_4}}^* \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle}{\langle 0 | \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle^2} - \frac{\langle 0 | \hat{n}_{\mathbf{q}_2, k_{z_3}} \hat{n}_{\mathbf{q}_2, k_{z_4}}^* | 0 \rangle \langle 0 | \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle}{\langle 0 | \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_1, k_{z_2}}^* | 0 \rangle^2} \right], \quad (18)
\end{aligned}$$

where  $\langle 0 | \hat{A} | 0 \rangle$  denotes the expectation value of an operator  $\hat{A}$  with respect to  $\Psi(0) = D$ . Following Gaskell, we use the following approximation:

$$\langle 0 | (\hat{n}_{\mathbf{q}, k_z} \hat{n}_{\mathbf{q}, k_z}^*)^2 | 0 \rangle = 2[\langle 0 | \hat{n}_{\mathbf{q}, k_z} \hat{n}_{\mathbf{q}, k_z}^* | 0 \rangle]^2 + \mathcal{O}(1/N) \quad (19)$$

and ignore correlations between different  $\hat{n}$ 's in the second term. The resulting approximation for  $I(\lambda)$  becomes

$$I(\lambda) = \frac{I(0)}{1 + \lambda I(0) 4u_{k_{z_1}, k_{z_2}}(\mathbf{q})}. \quad (20)$$

The corresponding approximation for the Fourier coefficients of the structure factor is obtained from the above equation for  $\lambda = 1$ , yielding

$$S_{k_{z_1}, k_{z_2}}(\mathbf{q}) = \frac{S_{k_{z_1}, k_{z_2}}^0(\mathbf{q})}{1 + 4u_{k_{z_1}, k_{z_2}}(\mathbf{q}) S_{k_{z_1}, k_{z_2}}^0(\mathbf{q})}. \quad (21)$$

### 2.2.2. Expectation value of the energy

In order to obtain the expression for the total energy of an inhomogeneous system we use the RPA approximation

$$\langle \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_2, k_{z_2}} \hat{n}_{\mathbf{q}_1 + \mathbf{q}_2, k_{z_3}} \rangle = \langle \hat{n}_{\mathbf{q}_1, k_{z_1}} \hat{n}_{\mathbf{q}_2, k_{z_2}} \rangle \langle \hat{n}_{\mathbf{q}_1 + \mathbf{q}_2, k_{z_3}} \rangle. \quad (22)$$

In the case of a system with density variation along  $z$  we have

$$\langle \hat{n}_{\mathbf{q}_1 + \mathbf{q}_2, k_z} \rangle = \begin{cases} V \rho_{k_z} & \text{if } \mathbf{q}_1 + \mathbf{q}_2 = 0, \\ 0 & \text{otherwise,} \end{cases} \quad (23)$$

where  $\rho_{k_z}$  represent the Fourier coefficients of the electronic density.

Making these assumptions and employing the expression for the structure factor obtained in the previous section, the terms  $\langle T_2 \rangle$  and  $\langle V_{ee} \rangle$  which appear in the expression for the total energy equation (4) can be written as

$$\begin{aligned}
\langle T_2 \rangle &= 2VN \sum_{\mathbf{q}_1, k_{z_1}, k_{z_2}, k_{z_3}, k_{z_4}} \hat{u}_{k_{z_1}, k_{z_2}}(q_1) \hat{u}_{k_{z_3}, k_{z_4}}(q_1) [(q_1)^2 - k_{z_1} k_{z_3}] \rho_{k_{z_1} + k_{z_3}}(S_{k_{z_2}, -k_{z_4}}(q_1)), \\
\langle V_{ee} \rangle &= n_0 \sum_{\mathbf{q}, k_z} \frac{2\pi}{(q^2 + k_z^2)^2} [(S_{k_z, -k_z}(q)) - 1]. \quad (24)
\end{aligned}$$

The above equation combined with our approximation (Eq. (21)) for the structure factor leads to an expression for the total energy in terms of the Fourier coefficients of the  $u$  function, the electron density and the non-interacting structure factor. We take both the density and non-interacting structure factor from

LDA calculations and minimize  $E$  with respect to the  $\hat{u}_{k_z, k_z'}(q)$  coefficients, which then can be used to construct the trial wave functions for VQMC calculations.

### 3. Results

This section presents the numerical results obtained for uniform and non-uniform spin-unpolarized  $N$ -electron systems ( $N = 38$ ) contained in a simple cubic (SC) simulation cell and satisfying periodic boundary conditions within the cell. Density modulations in  $z$  are induced by subjecting the system to an external potential of the form

$$V_{\text{ext}}(\mathbf{r}) = V_0 \cos(qz) \quad (25)$$

with  $V_0 = 0.1$  a.u.  $q = 0.6k_F$  is a reciprocal lattice vector of the SC simulation cell. The average density of the system corresponds to  $r_s = 2$ . The electron density is uniform in the  $x$ - $y$  plane and varies in the  $z$  direction.

The inhomogeneous  $u(\mathbf{r}_1, \mathbf{r}_2)$  term is represented by fixing the position  $\mathbf{r}_1$  of the first electron, while moving the second electron,  $\mathbf{r}_2$ , along the  $z$  direction on a line passing through  $\mathbf{r}_1$ .

#### 3.1. Homogeneous system

In Eq. (7) we saw that  $u(z_1, z_2)$  may be expanded as a Fourier series. In Fig. 1 the convergence of the energy with respect to the cutoff wavevector,  $k_{\text{cutoff}}$ , used in the Fourier expansion of the  $u$  factor is shown. The typical cutoff needed is small enough to be computationally feasible, so that such a representation for  $u(z_1, z_2)$  is found to be very useful.

Looking at the expression for the energy we see that for  $u(k) = 0$ ,  $\langle T_2 \rangle = 0$  and  $\langle V_{\text{ee}} \rangle$  is just the exchange energy of a HEG. For non-zero  $u(k)$  factors  $\langle T_2 \rangle + \langle V_{\text{ee}} \rangle$  includes both exchange and correlation energies. The correlation energy is defined as

$$E_c = [\langle T_2 \rangle + \langle V_{\text{ee}} \rangle] - [\langle T_2 \rangle + \langle V_{\text{ee}} \rangle]_{u(k)=0}. \quad (26)$$

Table 1 presents the values for the correlation energy obtained in this work in comparison with those obtained by Gaskell [1,2]. Differences due to finite size effects have to be taken into account, as we have considered a very small system with only  $N = 38$  electrons.

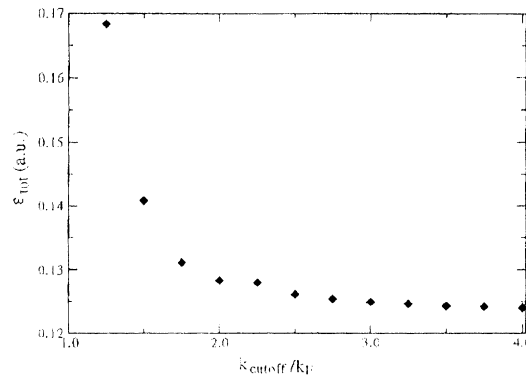


Fig. 1. The convergence of the total energy as a function of the cutoff  $k_{\text{cutoff}}$  used in the truncated Fourier series representation of the  $u$  function. The results are for  $N = 38$  and  $r_s = 2$ .  $k_{\text{cutoff}}$  is given in units of  $k_F$ .

Table 1  
Correlation energy per electron in a.u.

$r_s$	$\epsilon_c$	$\epsilon_c$ (Gaskell)
2	-0.04677	-0.058
3	-0.04175	-0.05
4	-0.03809	-0.0445
5	-0.0352	-0.0405

The results for the energy obtained with the uniform system previously described and using the homogeneous RPA  $u$  factor given in Section. 2.1 are presented in Table 2.

### 3.2. Inhomogeneous systems

The inhomogeneous RPA Jastrow factor considered here is the one derived in Section 2.2. The energies derived are presented in Table 2. Exchange-correlation energy is defined as

$$E_{xc} = \langle T_2 \rangle + \langle V_{ee} \rangle - E_H, \quad (27)$$

where  $E_H$  represents Hartree energy.

In Fig. 2(a) we plot the inhomogeneous RPA  $u$  term, for the three different positions of  $\mathbf{r}_1$  indicated in Fig. 2(b) which presents the LDA density and average electron density. The homogeneous Jastrow factor is shown as well, which depends only on the relative distance between the electrons and not their individual

Table 2  
Non-interacting kinetic energy  $\epsilon_{kin}^0 = (1/N) \sum_k k^2/2$ , exchange-correlation energy  $\epsilon_{xc} = E_{xc}/N$ , correlation energy  $\epsilon_c = E_c/N$  and total energy  $\epsilon_{tot} = E/N$  per electron in a.u. for (I) an uniform system using the homogeneous RPA  $u$  factor, (II) a weakly inhomogeneous system using the inhomogeneous RPA  $u$  factor. The cutoff wavevector used was equal to  $2.5k_F$

	$\epsilon_{kin}^0$	$\epsilon_{xc}$	$\epsilon_c$	$\epsilon_{tot}$
(I)	0.2807	-0.157	-0.04677	0.1235
(II)	0.2658	-0.1193	-0.0061	0.144

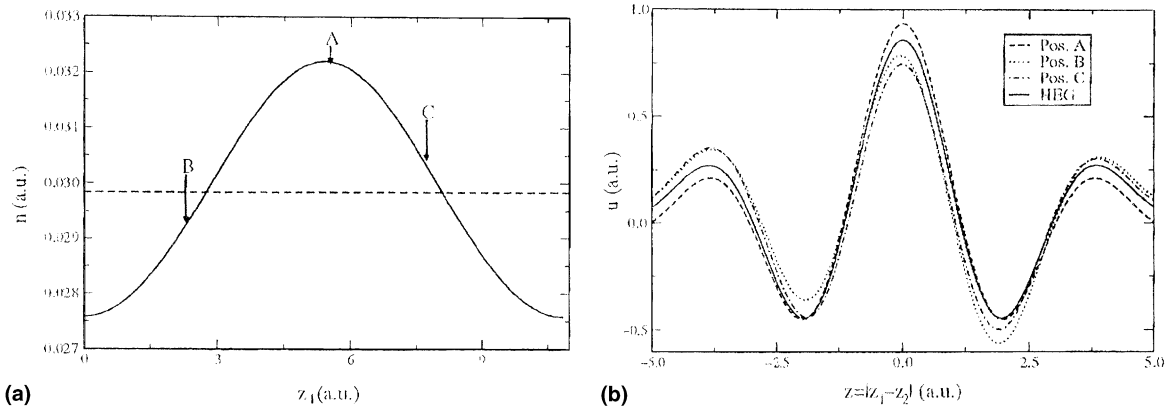


Fig. 2. (a) LDA electronic density of the system. The horizontal line represents the average electronic density of the system. (b) Inhomogeneous RPA  $u$  term for the three different positions of the fixed electrons shown in (a), together with the homogeneous result for the same system.

coordinates. Anisotropy of the Jastrow factor can be observed. This is such that the  $u$  function is stronger on the side where the density is lower. This can be explained by the fact that the RPA screening is more effective where the electron density is high, so that the  $u$  function is weaker on the high density side [12].

#### 4. Conclusions

We generalize the RPA treatment of the HEG by Gaskell to the inhomogeneous case. As a result we obtain a Slater–Jastrow trial wave function containing an anisotropic and inhomogeneous Jastrow factor. The latter may be obtained from the non-interacting structure factor and density of the system.

Results for the energy and the inhomogeneous correlation  $u$  factor using an electronic system subject to a sinusoidal external potential are presented. We compare these results with those obtained using the homogeneous  $u$  factor by Gaskell, and we clearly observe the anisotropy introduced by the inhomogeneous  $u$  factor. Future work will focus on testing the performance of our inhomogeneous Jastrow factor using variational Monte Carlo and in further refining our approximation of the interacting structure factor.

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