Many-Electron Trial Wave Functions for Inhomogeneous Solids

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Abstract

Quantum Monte Carlo simulations of interacting electrons in solids often use Slater-Jastrow trial wave functions with Jastrow factors containing one- and two-body terms. In uniform systems the long-range behavior of the two-body term may be deduced from the random-phase approximation (RPA) of Bohm and Pines. Here we generalize the RPA to nonuniform systems. This gives the long-range behavior of the inhomogeneous two-body correlation term and provides an accurate analytic expression for the one-body term. It also explains why Slater-Jastrow trial wave functions incorporating determinants of Hartree-Fock or density-functional orbitals are close to optimal even in the presence of an RPA Jastrow factor. After adjusting the inhomogeneous RPA Jastrow factor to incorporate the known short-range behavior, we test it using variational Monte Carlo calculations. We find that the most important

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aspect of the two-body term is the short-range behavior due to electron-electron scattering, although the long-range behavior described by the RPA should become more important at high densities.

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I. INTRODUCTION

This paper discusses approximate ground-state wave functions for inhomogeneous interacting many-electron systems such as solids. In particular, we consider wave functions of the Slater-Jastrow type, \( \Psi = e^J D \), where \( D \) is a Slater determinant and \( J \), the Jastrow factor, takes account of the electronic correlations. We have two main aims: we wish to devise a method for generating inhomogeneous Jastrow factors appropriate for use in strongly inhomogeneous solids; and we wish to understand the surprisingly accurate results obtained when Slater-Jastrow trial functions are used in variational (V) and diffusion (D) quantum Monte Carlo (QMC) simulations\(^1\) of weakly-correlated solids such as silicon. Despite the apparent simplicity of the Slater-Jastrow form, cohesive energies calculated using VQMC are typically an order of magnitude more accurate\(^3\)–\(^7\) than cohesive energies obtained using Hartree-Fock (HF) or density-functional theory within the local density approximation (LDA)\(^8\). Cohesive energies calculated using DQMC are even more accurate.

This is not the place for a general introduction to QMC (see Hammond et al.\(^9\) for a review), but a brief sketch of the VQMC method may be helpful. The idea is to obtain an approximate many-electron ground state by numerically optimizing an explicit parametrized trial wave function. Once this has been done, the calculation of expectation values reduces to the evaluation of multi-dimensional integrals. Ordinary integration methods using a grid become very inefficient when the dimension of the integral is greater than 5 or 10 (equivalent to a 2 or 3 electron system in three dimensions), and so the integrals are evaluated using Monte Carlo integration.\(^9\) This approach scales much more favorably with the dimension than grid-based integration methods.

The trial wave functions used in most QMC simulations contain a Slater determinant of LDA or HF orbitals and a Jastrow factor that includes pairwise correlation terms, \( u_{\sigma_i \sigma_j}(r_i, r_j) \), and one-electron terms, \( \chi_{\sigma_i}(r_i) \), where \( r_i \) and \( \sigma_i \) are the position and spin component of electron \( i \). The \( u \) and \( \chi \) functions are usually obtained by optimizing specific parametrized functional forms according to the variational principle. In simulations of
solids, it is common to simplify the optimization by insisting that \( u \) be both homogeneous and isotropic (i.e., \( u_{\sigma_i,\sigma_j}(r_i, r_j) \) is assumed to depend only on the interelectronic distance \( r_{ij} = |r_i - r_j| \)).

By contrast, our principal aim is to derive a physically-motivated inhomogeneous and anisotropic Jastrow factor for nonuniform systems, based on a generalization of the random-phase approximation (RPA) of Bohm and Pines. This will enable us to reduce or even dispense with the time-consuming optimization procedure. The RPA is known to give unphysical results in some cases and is not generally regarded as an accurate quantitative method. Here, however, we use the RPA only to guide the construction of an approximate trial wave function. Once this wave function has been chosen, energies are calculated using the true interacting many-electron Hamiltonian instead of the approximate RPA form. The results are therefore variational and much more accurate than standard RPA energies.

The RPA theory of the homogeneous electron gas is already used in the construction of Jastrow factors for QMC simulations. This approach predicts that the \( u \) function should decay like \( 1/r_{ij} \) for large \( r_{ij} \), but says nothing about the \( \chi \) function (which is zero in a homogeneous system) or the short-range behavior of \( u \). Although it is easy to modify the \( u \) function to make it have the correct cusp-like behavior at short range, the absence of \( \chi \) terms implies that the homogeneous RPA Jastrow factor produces inaccurate densities, and hence poor energies, when used in strongly inhomogeneous systems. This problem is usually fixed by adding a parametrized \( \chi \) function and optimizing the parameters numerically.

Here, we generalize the RPA theory to inhomogeneous systems (see Malatesta and Fahy for an alternative approach). We obtain a correlation term that is truly inhomogeneous and anisotropic. Furthermore, as originally noted by Malatesta et al., we find that the inhomogeneous RPA theory automatically produces a Jastrow factor containing \( \chi \) terms. The short-range behavior of the inhomogeneous RPA \( u \) function is no better than that of the homogeneous version but is more difficult to correct. We impose the required short-range cusps using a \( k \)-space method which, although approximate, works well.

An interesting aspect of the inhomogeneous RPA theory is that it provides a justification
for using Slater determinants consisting of LDA or HF orbitals. This is common practice but is not obviously correct: one might guess that the HF orbitals that are optimal in the absence of a Jastrow factor would no longer be accurate in its presence. In fact, the RPA theory shows that HF or LDA orbitals are close to optimal whether or not an RPA Jastrow factor is present.

We test our inhomogeneous RPA Jastrow factor by carrying out VQMC calculations for a strongly inhomogeneous electron gas. We find that the inhomogeneous RPA $\chi$ functions are of such high quality that there is no need to resort to the standard but costly numerical optimization methods. Surprisingly, however, we gain almost no advantage by using inhomogeneous $u$ functions: a Jastrow factor consisting of a homogeneous $u$ function plus any good $\chi$ function gives almost the same results. Inhomogeneous $u$ functions are often used in full core atomic and molecular calculations but do not seem necessary in the strongly inhomogeneous electron gases studied here. Some recent VQMC simulations by Hood and Nekovee suggest a possible explanation for this observation. Although our system has a strongly inhomogeneous exchange-correlation hole $n_{xc}(r, r') = [g(r, r') - 1]n(r')$, the LDA seems to provide a better description of the pair-correlation function $g(r, r')$. The use of a strongly inhomogeneous $u$ function may therefore be unnecessary.

In agreement with previous work we conclude that the most important features of the Jastrow factor are (i) that the corresponding Slater-Jastrow wave function produces an accurate electron density, and (ii) that the $u$ function has the correct cusp-like behavior whenever two electrons approach each other. As long as both these conditions are satisfied, the calculated energies are normally quite accurate.

In summary, the five main results of our paper are:

1. We have extended the RPA to inhomogeneous systems.

2. We have used the inhomogeneous RPA theory to derive expressions for the $\chi$ function and for the long-range behaviour of the fully inhomogeneous $u$ function.
3. We have developed a general method for imposing a cusp on any inhomogeneous Jastrow factor expressed in $k$-space.

4. The inhomogeneous RPA analysis has enabled us to explain why Slater-Jastrow-type wave functions containing LDA or HF orbitals work so well.

5. We have implemented and tested the inhomogeneous RPA Jastrow factor and found that the calculated one-body term works perfectly, but that the inhomogeneity of the two-body term contributes little to the energy at typical valence electron densities.

The rest of this paper is organized as follows. In Sec. II we describe the Slater-Jastrow trial wave functions used in most QMC simulations of atoms, molecules, and solids. Section III presents the RPA theory of the inhomogeneous electron gas and explains how it leads to Slater-Jastrow trial wave functions containing both $\chi$ terms and inhomogeneous $u$ terms. To supplement the somewhat mathematical presentation in Sec. III, Appendix A describes the RPA in more physical terms. Section IV discusses the results of the VQMC simulations we have done to test the inhomogeneous RPA Jastrow factor, and Sec. V concludes.

II. TRIAL WAVE FUNCTIONS FOR QMC SIMULATIONS

The aim of this paper is to provide a better physical understanding of the success of the Slater-Jastrow trial wave functions used in many QMC calculations of atoms, molecules, and weakly correlated solids. A Slater-Jastrow trial function is the product of a totally antisymmetric Slater determinant $D$ and a totally symmetric Jastrow factor $e^J$. The Slater determinant is often split into two smaller determinants, one for each spin value:

$$\Psi = e^J D_\uparrow D_\downarrow .$$

This spoils the antisymmetry of the trial wave function on interchange of electrons of opposite spin, but does not affect expectation values of spin-independent operators. Since two smaller determinants are easier to deal with than one big one, it also reduces the numerical
complexity of the problem. The orbitals used in $D_↑$ and $D_↓$ are normally obtained from LDA or HF calculations.

The Slater determinants build in exchange effects but neglect 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 a pairwise Jastrow factor of the form,

$$ J = \frac{1}{2} \sum_{i,j} u_{\sigma_\sigma}(r_i, r_j), \quad (2.2) $$

where $u_{\sigma\sigma'}(r, r') = u_{\sigma'\sigma}(r', r)$. Because the LDA or HF orbitals in $D_↑$ and $D_↓$ already give a reasonably good approximation to the density, the introduction of a two-body $u$ function usually causes the density of the many-electron wave function to deteriorate. As a result the trial energy deteriorates too. It is therefore necessary to introduce one-body $\chi$ terms to adjust the Jastrow factor:

$$ e^J = \exp \left( \frac{1}{2} \sum_{i,j} u_{\sigma_\sigma}(r_i, r_j) + \sum_i \chi_\sigma(r_i) \right). \quad (2.3) $$

Note the sign conventions here: our definition of $u$ is the negative of that used by many other authors. Most authors also omit the diagonal $i = j$ terms in the sum over $i$ and $j$, but we find it mathematically convenient to include them in our analysis. In homogeneous systems the diagonal terms only affect the normalization of the trial function, while in inhomogeneous systems they add one-body contributions that may be accounted for by a simple redefinition of $\chi_\sigma(r)$.

Since we are using periodic boundary conditions, it will often prove convenient to express the electron density and Jastrow factor in reciprocal space:

$$ n_\sigma(k) = \frac{1}{\sqrt{V}} \int_V n_\sigma(r) e^{ik \cdot r} d^3r, \quad (2.4) $$

$$ \chi_\sigma(k) = \frac{1}{\sqrt{V}} \int_V \chi_\sigma(r) e^{ik \cdot r} d^3r, \quad (2.5) $$

$$ u_{\sigma\sigma'}(k, k') = \frac{1}{V} \int_V e^{i k \cdot r} u_{\sigma\sigma'}(r, r') e^{-i k' \cdot r'} d^3r d^3r'. \quad (2.6) $$
Note that we are using a symmetric definition of the Fourier transformation; the corresponding back transformation is \( f(r) = V^{-1/2} \sum_k f(k)e^{-ir\cdot k} \).

Several different types of Jastrow factor are in common use:

1. Jastrow factors based on the RPA theory of the uniform electron gas in the form due to Bohm and Pines. In this paper we show how to generalization this approach to obtain Jastrow factors for strongly inhomogeneous systems.

2. Jastrow factors based on the RPA theory of the uniform electron gas in the form due to Gaskell. This type of Jastrow factor has been widely used by Ceperley and coworkers.

3. Jastrow factors obtained by the numerical optimization of a parametrized functional form. In most cases the optimization is carried out using the variance minimization technique in the form developed by Umrigar.

4. Jastrow factors derived using the Fermi hypernetted chain approximation as given by Krotscheck et al.

A. The cusp conditions

In this section we deduce the short-range behavior of \( u \). When the distance \( r_{ij} = |r_i - r_j| \) between two electrons approaches zero, the potential energy in the Hamiltonian operator diverges like \( 1/r_{ij} \). (Except where otherwise stated, we use Hartree atomic units, \( \hbar = e = 4\pi\varepsilon_0 = m_e = 1 \), throughout this paper.) Since, for any exact eigenstate, \( \hat{H}\Psi \) is proportional to \( \Psi \), this Coulomb divergence must be cancelled by an equal and opposite divergence in the kinetic energy terms. When choosing a trial wave function for use in a QMC simulation, it is important to ensure that this exact cancellation still occurs. If it does not, the local energy \( E_L = \hat{H}\Psi/\Psi \), which is the quantity actually sampled in the simulation, diverges as \( r_{ij} \) approaches zero, causing numerical difficulties.
Since, away from the nuclei, the single-particle orbitals are smooth functions of the electronic coordinates, the determinantal part of the trial wave function depends smoothly on the positions of the electrons. For small $r_{ij}$, it may therefore be expanded in the form:

$$(D_\uparrow D_\downarrow)|_{r_{ij}\to 0} = c + a \cdot r_{ij} + \ldots .$$

The application of the kinetic energy operator to this series produces a smooth function of $r_{ij}$, whereas the application of the potential energy operator places a divergent $1/r_{ij}$ factor in front of every term.

It is clear that a trial function containing only the Slater determinants does not show the required cancellation of potential and kinetic energy divergences. The cancellation may however be imposed by modifying the terms of the expansion as follows:

$$
\begin{align*}
c & \to (1 + \frac{1}{2}r_{ij}) c , \\
a \cdot r_{ij} & \to (1 + \frac{1}{4}r_{ij}) a \cdot r_{ij} .
\end{align*}
$$

Each term in the series is multiplied by a factor, $1 + \alpha r_{ij}$, which includes a cusp at $r_{ij} = 0$. The numerical constant $\alpha$ in front of the cusp is $1/(2 + 2n)$, where $n$ is the order of $r_{ij}$ in the original expansion.

A convenient way to introduce a cusp-like term is to include it in the Jastrow factor $e^J$ in such a way that the cusp terms $(1 + \frac{1}{2}r_{ij})$ or $(1 + \frac{1}{4}r_{ij})$ appear in the expansion of $e^J$ for small $r_{ij}$. As we only have one Jastrow factor we can only hope to deal with one of the terms in the expansion of $D_\uparrow D_\downarrow$ correctly; we choose the lowest order term that is nonzero, as this is the one that causes the divergence in the local energy $E_L$. If electrons $i$ and $j$ have antiparallel spins, the lowest order term is the constant $c$; for parallel spins, $D_\uparrow D_\downarrow$ is an antisymmetric function of $r_{ij}$ and so the lowest order term is $a \cdot r_{ij}$. The required cusp may thus be introduced by imposing the following conditions on $u_{\sigma_i\sigma_j}$:

$$
\frac{\partial u_{\uparrow\downarrow}}{\partial r_{ij}}|_{r_{ij}=0} = \frac{1}{2}
$$

for antiparallel spins, and

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\[
\frac{\partial u_{\uparrow\uparrow}(\mathbf{r}_i, \mathbf{r}_j)}{\partial r_{ij}} \bigg|_{r_{ij}=0} = \frac{1}{4}
\]  
(2.10)

for parallel spins.  

B. The homogeneous RPA correlation term

As will be explained in Sec. [3], the RPA theory of Bohm and Pines [3] suggests that the long-range behavior of the correlation term \(u\) in a homogeneous electron gas of number density \(n\) should take the form:

\[
u_{\sigma_i \sigma_j}(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{\omega_p r_{ij}},
\]  
(2.11)

where \(\omega_p = \sqrt{4\pi n}\) is the plasma frequency. This spin-independent two-body term has no cusp and is only expected to be correct for large \(r_{ij}\). Multiplying Eq. (2.11) by \(1 - e^{-r_{ij}/F_{\sigma_i \sigma_j}}\) yields

\[
u_{\sigma_i \sigma_j}(r_{ij}) = -\frac{1}{\omega_p r_{ij}} \left(1 - e^{-r_{ij}/F_{\sigma_i \sigma_j}}\right),
\]  
(2.12)

which approaches Eq. (2.11) for large \(r_{ij}\) and also has the correct cusp behavior if \(F_{\sigma_i \sigma_j}\) is chosen appropriately. Because of the spin dependence of the cusp conditions, we need different values of \(F\) for parallel- and antiparallel-spin electrons. By expanding Eq. (2.12) to first order in \(r_{ij}\), we see that the cusp conditions Eq. (2.9) and Eq. (2.10) become

\[
\frac{1}{2} = \frac{du_{\uparrow\downarrow}}{dr} \bigg|_{r=0} = \frac{1}{2F_{\uparrow\downarrow}^2 \omega_p}
\]  
(2.13)

for antiparallel spins, and

\[
\frac{1}{4} = \frac{du_{\uparrow\uparrow}}{dr} \bigg|_{r=0} = \frac{1}{2F_{\uparrow\uparrow}^2 \omega_p}
\]  
(2.14)

for parallel spins.
C. The $\chi$ function

The $\chi$ function needed to counteract the density-adjusting effects of the $u$ function is normally obtained by numerical optimization. If we wish to avoid this costly procedure we have several options:

1. We could use no one-body term and hope for the best. This is the correct thing to do in a homogeneous system and also proves satisfactory in cases when the spatial variation of the charge density is much more rapid than that of the $u$ function.

2. We could use the result of Sec. III and include a one-body term of the form:

$$\chi_\sigma(k) = - \sum_{k',\sigma'} u_{\sigma\sigma'}(k,k') n_{\sigma'}(k').$$

(2.15)

3. We could use a one-body term as given by Malatesta et al.:

$$\chi_\sigma(k) = - \sqrt{V} \sum_\sigma u_{\sigma\sigma'}(k) n_{\sigma'}(k).$$

(2.16)

In cases when the $u$ function is homogeneous,

$$u_{\sigma\sigma'}(r,r') = u_{\sigma\sigma'}(r-r'),$$

(2.17)

we get

$$u_{\sigma\sigma'}(k,k') = \sqrt{V} u_{\sigma\sigma'}(k) \delta_{k,k'}$$

(2.18)

and so Eq. (2.15) reduces to Eq. (2.16). Option (2) therefore reduces to option (3). Strictly speaking, however, $u$ is never exactly homogeneous unless the electron density is exactly uniform, in which case both options (2) and (3) merely state that $\chi = 0$. 

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III. THE RANDOM-PHASE APPROXIMATION FOR INHOMOGENEOUS SYSTEMS

This section starts with a brief introduction to the ideas behind the standard RPA treatment of homogeneous systems. We then generalize the RPA theory to inhomogeneous systems. This generalization shows us how to construct approximate ground-state wave functions of the Slater-Jastrow type. The RPA forms of the $u$ and $\chi$ functions are closely related and both depend on the electron density.

A. Review of the RPA for homogeneous systems

Let us first give a brief overview of the standard RPA as formulated for homogeneous systems. The starting point is the usual Hamiltonian,

$$\hat{H} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_k \hat{n}_k \hat{n}_k^\dagger - \frac{2\pi N}{V} \sum_k \frac{1}{k^2}, \quad (3.1)$$

of a uniform electron gas in a volume $V$. Note that we have adopted a slightly unusual definition of the number density operator,

$$\hat{n}_k = \frac{1}{\sqrt{V}} \sum_i e^{ik\cdot\hat{r}_i}, \quad (3.2)$$

which includes a $1/\sqrt{V}$ factor in order to be consistent with the symmetric definition of the Fourier transform used throughout this paper. The $k$-points are chosen in accordance with the geometry of the system, which is taken to obey periodic boundary conditions. The system is assumed to be charge neutral and so the $k = 0$ terms are omitted from the $k$-space summations.

As we are interested in describing the long-range correlations due to the electron-electron interaction, we wish to make a connection between the Hamiltonian of Eq. (3.1) and the long wavelength density fluctuations known as plasmons. Our eventual aim is to split the Hamiltonian into an electronic term with short-range interactions and a plasmon term that
is only weakly coupled to the electrons. Once the electron and plasmon parts of the Hamiltonian have been (almost) decoupled in this way, we shall see that the long-range correlations are described by the ground-state wave function of the plasmon part, which is simply a set of quantum mechanical harmonic oscillators. At shorter wavelengths the plasmons are not well defined and the collective plasmon description of electronic correlation ceases to be valid. Instead, the electrons feel a short-range screened interaction that produces additional electron-electron scattering-like correlations.

The assumption of weak plasmon-electron interaction is reasonable at small $k$ since long wavelength plasmons are long lived. For larger $k$ values, however, the almost flat plasmon dispersion curve runs into the continuum of electron-hole pair excitations and the plasmons are no longer well defined. In a uniform electron gas this happens at a wave vector $k_c$ given by

$$
k_c \approx \frac{1}{2} k_F r_s^{1/2} \propto n^{1/6}, \quad (3.3)$$

where $k_F$ is the Fermi wave vector, $r_s a_0$ is the radius of a sphere containing one electron on average, and $a_0$, the Bohr radius, is the atomic unit of length. This estimate of the cutoff should also be applicable to inhomogeneous systems as long as the density does not vary too much. We see that for typical metals with $r_s$ values of 2 or 3 the cutoff is of the order of the Fermi wave vector. We also see that the higher the density the better the plasmon description should be. The inverse of $k_c$ is a measure of the minimum length scale on which the electronic correlations may be described in terms of plasmons.

The first step in the derivation of the homogeneous RPA is to introduce a new pair of conjugate operators, $\hat{\pi}_k$ and $\hat{q}_k$, for every wave vector $k$ with modulus $k < k_c$. These operators act in a new Hilbert space that we call the oscillator space, and transform like $\hat{n}_k$ under Hermitian conjugation: $\hat{n}_k = \hat{\pi}_k^\dagger$ and $\hat{q}_k = \hat{q}_k^\dagger$. The physical and oscillator Hilbert spaces are quite distinct, and so $\hat{n}_k$ and $\hat{q}_k$ commute with $\hat{r}_i$ and $\hat{p}_i$. For the time being $\hat{n}_k$ and $\hat{q}_k$ have little physical meaning, but later in the derivation they will become associated with the plasmon coordinates.
The oscillator-space operators are now used to define a new Hamiltonian,
\[
\hat{H}_{BP} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_k \frac{\hat{n}_k \hat{n}_k^\dagger}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2} \\
+ \frac{1}{2} \sum_{k<k_c} \hat{n}_k \hat{n}_k^\dagger - \sum_{k<k_c} \left( \frac{4\pi}{k^2} \right)^{1/2} \hat{n}_k \hat{n}_k^\dagger,
\]
which acts in an enlarged Hilbert space that is the product of the physical space and the oscillator space. The Bohm-Pines Hamiltonian \(\hat{H}_{BP}\) may be written in the form
\[
\hat{H}_{BP} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_{k>k_c} \frac{\hat{n}_k \hat{n}_k^\dagger}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2} \\
+ \frac{1}{2} \sum_{k<k_c} \left( \frac{4\pi}{k^2} \right)^{1/2} \hat{n}_k \hat{n}_k^\dagger,
\]
and so its eigenvalue spectrum is bounded below.

We now restrict our attention to those states \(|\Phi\rangle\) from the enlarged Hilbert space that satisfy the subsidiary condition:
\[
\hat{n}_k |\Phi\rangle = 0 \text{ for all } k < k_c.
\]
Any state obeying Eq. (3.6) may be written in the form \(|\Phi\rangle = |\psi\rangle |\pi=0\rangle\), where \(|\psi\rangle\) is a state in the physical Hilbert space and \(|\pi=0\rangle\) is the oscillator-space state satisfying
\[
\hat{n}_k |\pi=0\rangle = 0 \text{ for all } k < k_c.
\]
(The bold symbol \(\pi\) is shorthand for the vector of all the \(\pi_k\) with \(k < k_c\).) The set of product-space states satisfying the subsidiary condition may therefore be put into one-to-one correspondence with the set of physical states. Equally, given any eigenstate \(|\psi\rangle\) with eigenvalue \(E\) of the original Hamiltonian, the product state \(|\Phi\rangle = |\psi\rangle |\pi=0\rangle\) satisfies the subsidiary condition, Eq. (3.6), and is an eigenstate of Eq. (3.4) with the same energy. This is because all the new terms in \(\hat{H}_{BP}\) involve \(\hat{n}_k\) and hence give zero when operating on \(|\pi=0\rangle\).
As long as the subsidiary condition is obeyed, the additional degrees of freedom may simply be regarded as dummy variables, both in the wave function and the Hamiltonian.

It will be proved later on in this paper that the overall ground state \(|\Phi_0\rangle\) of the extended Hamiltonian, Eq. (3.4), automatically satisfies the subsidiary condition, Eq. (3.6).
The physical-space part of the ground state of $\hat{H}_{BP}$ is therefore the ground state of the original Hamiltonian, and we might as well study the ground-state properties of the extended Hamiltonian as those of the original.

The next stage in the derivation is to make a unitary transformation, which will be described in more detail in Sec. III C. Once the extended Bohm-Pines Hamiltonian has been transformed and several supposedly small terms have been dropped, the transformed Hamiltonian may be written as the sum of a spatial Hamiltonian with a short-range interaction,

$$\hat{H}_{sr} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_{k > k_c} \frac{\hat{n}_k \hat{n}_k^\dagger}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2}, \quad (3.8)$$

and an oscillator-like plasmon term,

$$\hat{H}_p = \frac{1}{2} \sum_{k < k_c} \left( \hat{\pi}_k \hat{\pi}_k^\dagger + \omega_p^2 \hat{q}_k \hat{q}_k^\dagger \right), \quad (3.9)$$

where $\omega_p = (4\pi N/V)^{1/2}$ is the plasma frequency. One of the approximations made during the derivation of these results involves the replacement of an exponential factor of the form $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \hat{\mathbf{r}}_i]$ by its average value. Since the electronic positions $\mathbf{r}_i$ are effectively random in a homogeneous system, the phase of the exponential is also random unless $\mathbf{k} = \mathbf{k}'$, and so the average is 1 if $\mathbf{k} = \mathbf{k}'$ or zero otherwise. This is the eponymous random-phase approximation.

The approximate Hamiltonian,

$$\hat{H}_{RPA} = \hat{H}_{sr} + \hat{H}_p, \quad (3.10)$$

still includes short-range electron-electron interactions and so cannot be solved exactly. We may, however, use the HF method or the LDA to obtain approximate eigenstates of $\hat{H}_{sr}$. These approximate eigenstates, which are of course Slater determinants, may then be multiplied by eigenstates of the oscillator Hamiltonian, Eq. (3.9), to obtain approximate eigenstates of the full Hamiltonian $\hat{H}_{RPA}$. The unitary transformation may then be inverted to obtain approximate eigenstates of $\hat{H}_{BP}$. Unlike the exact ground state, the resulting approximate ground state of $\hat{H}_{BP}$ does not satisfy the subsidiary condition, Eq. (3.6), exactly. It
may, however, be projected onto the subspace of states that do satisfy the subsidiary condition to obtain an approximate ground state in the physical Hilbert space. This approximate physical ground state has the homogeneous Slater-Jastrow form,

$$\psi_0(\{x_i\}) = \exp\left[-\frac{2\pi}{\omega_p} \sum_{k<k_c} \frac{n_k \hat{n}^\dagger_k}{k^2}\right] D(\{x_i\}) , \quad (3.11)$$

where $n_k = V^{-1/2} \sum_i e^{ik \cdot r_i}$ and $x_i = (r_i, \sigma_i)$ describes the position and spin component of electron $i$. The RPA $u$ function is therefore independent of spin and proportional to $1/r_{ij}$ at large $r_{ij}$. As noted earlier, the cutoff wave vector $k_c$ is usually chosen to be of the order of the Fermi wave vector $k_F$.

**B. The RPA Hamiltonian in inhomogeneous systems**

The aim is to find an approximate ground state $|\psi_0\rangle$ with energy $E_0$ of the following Hamiltonian:

$$\hat{H} = \frac{1}{2} \sum_i \hat{p}_i^2 + \sum_i V(\hat{r}_i)$$

$$+ 2\pi \sum_k \frac{\hat{n}_k \hat{n}^\dagger_k}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2} , \quad (3.12)$$

where $V(\mathbf{r})$ is an applied potential. The “physical” Hilbert space in which this Hamiltonian acts will be denoted $\mathcal{H}_R$. For reasons that will become clear later on, it is sometimes convenient to rewrite $\hat{H}$ in the form,

$$\hat{H} = \frac{1}{2} \sum_i \hat{p}_i^2 + \sum_i \tilde{V}(\hat{r}_i)$$

$$+ 2\pi \sum_k \frac{\hat{n}_k \hat{n}^\dagger_k}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2}$$

$$+ \frac{1}{2} \sum_{k<k_c} \hat{n}^0_{k} \hat{n}^0_{-k} - \sum_{k<k_c} \left(\frac{4\pi}{k^2}\right)^{1/2} \hat{n}_k \hat{n}^\dagger_k , \quad (3.13)$$

where $\tilde{V}(\mathbf{r})$ is defined via:
\[ \tilde{V}(\mathbf{r}) = V(\mathbf{r}) - \frac{\Delta E}{N} - \Delta V(\mathbf{r}) , \]  
(3.14)

\[ \Delta E = \frac{1}{2} \sum_{k<k_c} \pi_k^0 \pi_{-k}^0 , \]  
(3.15)

\[ \Delta V(\mathbf{r}) = - \sum_{k<k_c} \left( \frac{4\pi}{k^2} \right)^{1/2} \frac{\pi_k^0}{\sqrt{V}} e^{-ik\cdot\mathbf{r}} , \]  
(3.16)

and the \( \pi_k^0 \) are arbitrary numbers satisfying \( \pi_{k}^{0*} = \pi_{-k}^0 \).

Let us now introduce conjugate pairs of operators, \( \hat{\pi}_k \) and \( \hat{q}_k \), acting in a different Hilbert space \( \mathcal{H}_O \), which we call the oscillator space. The “momentum” operator \( \hat{\pi}_k \) and the “position” operator \( \hat{q}_k \) are taken to be the Fourier transforms of field operators \( \hat{\pi}(\mathbf{r}) = \hat{\pi}^\dagger(\mathbf{r}) \) and \( \hat{q}(\mathbf{r}) = \hat{q}^\dagger(\mathbf{r}) \):

\[ \hat{q}_k^\dagger = \frac{1}{\sqrt{V}} \int_V e^{ik\cdot\mathbf{r}} \hat{q}^\dagger(\mathbf{r}) d^3r , \]  
(3.17)

\[ \hat{\pi}_k = \frac{1}{\sqrt{V}} \int_V e^{ik\cdot\mathbf{r}} \hat{\pi}(\mathbf{r}) d^3r , \]  
(3.18)

which satisfy the commutation relation

\[ [\hat{\pi}(\mathbf{r}), \hat{q}(\mathbf{r}')] = -i\delta(\mathbf{r} - \mathbf{r}') . \]  
(3.19)

It therefore follows that \( \hat{\pi}_k^\dagger = \hat{\pi}_{-k} \) and \( \hat{q}_k^\dagger = \hat{q}_{-k} \) obey

\[ [\hat{\pi}_k, \hat{q}_k] = -i\delta_{k,k'} . \]  
(3.20)

We can form an extended Hilbert space by taking the product space \( \mathcal{H}_{ext} = \mathcal{H}_R \otimes \mathcal{H}_O \). If we denote the identity operators in the real and oscillator spaces by \( \hat{1}_R \) and \( \hat{1}_O \) respectively, we can define extended-space operators such as \( \hat{r}_{ext} = \hat{r}_R \otimes \hat{1}_O \) and \( \hat{q}_{ext} = \hat{1}_R \otimes \hat{q}_O \) corresponding to any operator belonging to one or other of the constituent Hilbert spaces. It is obvious that all the extended “\( R \)” operators commute with all the extended “\( O \)” operators. From now on we shall omit the identity operators and drop all “\( O \)”, “\( R \)”, and “\( ext \)” subscripts. Operators will always be denoted using hats, and so anything without a hat may be assumed to be a (possibly complex) number.
Now consider the Hermitian extended Hamiltonian,

\[
\hat{H}_{BP} = \frac{1}{2} \sum_i \hat{p}_i^2 + \sum_i \tilde{V}(\hat{r}_i) + 2\pi \sum_k \hat{n}_k \hat{n}_k^\dagger - \frac{2\pi N}{k^2} \sum_k \frac{1}{k^2} + \frac{1}{2} \sum_{k<k_c} \hat{n}_k \hat{n}_k^\dagger - \sum_{k<k_c} (\frac{4\pi}{k^2})^{1/2} \hat{n}_k \hat{n}_k^\dagger,
\]

which is an operator in the extended Hilbert space \(H_{ext}\). Note that the potential \(\tilde{V}\) is still the same as given by Eq. (3.14); the variables \(\pi_k^0\) that were used to construct \(\tilde{V}\) have not been replaced by operators in \(H_O\), but remain ordinary complex numbers. Because \(\hat{H}_{BP}\) and \(\tilde{\pi}\) commute they may be diagonalized simultaneously, and hence all eigenstates of the extended Hamiltonian \(\hat{H}_{BP}\) may be written in the form \(|\psi_\pi\rangle|\pi\rangle\), where \(\pi_k|\pi\rangle = \pi_k|\pi\rangle\) for all \(k < k_c\).

Let \(|\psi_0\rangle\) and \(E_0\) be the ground-state wave function and ground-state eigenvalue of the physical Hamiltonian \(\hat{H}\). If we define an eigenstate \(|\pi^0\rangle\) of the \(\pi_k\) operators such that \(\pi_k|\pi^0\rangle = \pi_k^0|\pi^0\rangle\) for all \(k < k_c\), it follows that \(|\psi_0\rangle|\pi^0\rangle\) is an eigenstate of \(\hat{H}_{BP}\) with the same eigenvalue \(E_0\). It need not, however, be the ground state of \(\hat{H}_{BP}\), which might correspond to a different wave function \(|\psi_{\pi_{\text{min}}}\rangle|\pi_{\text{min}}\rangle\). The question that now arises is how to choose the constants \(\pi_k^0\) (and hence the modified potential \(\tilde{V}\)) such that \(|\psi_0\rangle|\pi^0\rangle\) is in fact the ground state of \(\hat{H}_{BP}\) and not just some other eigenstate. In other words, we have to find a link between the \(\pi_k^0\) and \(|\psi_0\rangle\). This can be achieved using the Hellmann-Feynman theorem.

Consider the lowest energy state \(|\Phi_\pi\rangle = |\psi_\pi\rangle|\pi\rangle\) corresponding to some fixed oscillator-space eigenstate \(|\pi\rangle\). The energy eigenvalue of \(|\Phi_\pi\rangle\) will be denoted \(E^\pi\). When \(\hat{H}_{BP}\) acts on \(|\Phi_\pi\rangle\), the operators \(\pi_k\) may be replaced by their eigenvalues \(\pi_k\), and hence \(|\psi_\pi\rangle\) is in fact the ground state of

\[
\hat{H}^\pi = \frac{1}{2} \sum_i \hat{p}_i^2 + \sum_i \tilde{V}(\hat{r}_i) + 2\pi \sum_k \hat{n}_k \hat{n}_k^\dagger - \frac{2\pi N}{k^2} \sum_k \frac{1}{k^2},
\]
\[ + \frac{1}{2} \sum_{k < k_c} \pi_k \pi_{-k} - \sum_{k < k_c} \left( \frac{4\pi}{k^2} \right)^{1/2} \pi_k \hat{n}_k^\dagger. \] (3.22)

Note that \( \hat{H}^\pi \) operates not in the extended Hilbert space but in \( \mathcal{H}_R \). Furthermore, it is important to keep in mind that \( \tilde{V} \) is formed using the as yet unknown numbers \( \pi_0^k \). The overall ground state of \( \hat{H}_{BP} \) corresponds to the minimum of \( E^\pi \) with respect to \( \pi \). As we are now looking at a standard quantum mechanical problem formulated in the physical Hilbert space \( \mathcal{H}_R \), the Hellmann-Feynman theorem gives:

\[
\frac{\partial E^\pi}{\partial \pi_k} = \left( \psi_\pi | \frac{\partial \hat{H}^\pi}{\partial \pi_k} | \psi_\pi \right) = \pi_{-k} - \left( \frac{4\pi}{k^2} \right)^{1/2} \langle \psi_\pi | \hat{n}_k^\dagger | \psi_\pi \rangle, \quad (3.24)
\]

where \( |\psi_\pi\rangle \) is assumed normalized. If the overall ground state of \( \hat{H}_{BP} \) occurs when \( \pi = \pi_{\text{min}} \), it follows that:

\[
0 = \pi_{-k} - \left( \frac{4\pi}{k^2} \right)^{1/2} \langle \psi_{\pi_{\text{min}}} | \hat{n}_k^\dagger | \psi_{\pi_{\text{min}}} \rangle. \quad (3.25)
\]

We wish to choose the constants \( \pi_0^k \) such that \( \pi_0^k = \pi_{\text{min}}^k \), since in this case we have already argued that the physical-space part \( |\psi_{\pi_0}\rangle \) of the Bohm-Pines ground state

\[
|\Phi_{\pi_0}\rangle = |\psi_{\pi_0}\rangle |\pi_0\rangle \quad (3.26)
\]
is equal to the exact physical ground state \( |\psi_0\rangle \). The sought after link between \( |\psi_0\rangle \) and the \( \pi_0^k \) is therefore:

\[
\pi_0^k = \left( \frac{4\pi}{k^2} \right)^{1/2} \langle \psi_0 | \hat{n}_k^\dagger | \psi_0 \rangle = \left( \frac{4\pi}{k^2} \right)^{1/2} \langle \hat{n}_{-k} \rangle_0, \quad (3.27)
\]

where \( \langle \hat{n}_k \rangle_0 = \langle \psi_0 | \hat{n}_k | \psi_0 \rangle \) is a Fourier component of the ground-state electron density \( n(r) \).

Note that Eq. (3.27) is not an operator equation; it simply links one number, \( \pi_{-k}^0 \), to another, \( \langle \hat{n}_{-k} \rangle_0 \). Since all the \( \hat{n}_k \) operators have \( k < k_c \), Eq. (3.27) only applies when \( k < k_c \).

We still have to verify that the stationary point \( \pi_{\text{min}} \) is in fact the minimum of \( E^\pi \). Eq. (3.24) determines the slope at any given \( \pi \). The matrix of second derivatives of \( E^\pi \), which determines the curvature, may therefore be obtained by differentiating Eq. (3.24):
\[
\frac{\partial}{\partial \pi_{-k'}} \frac{\partial}{\partial \pi_k} E^\pi = \delta_{-k,-k'} + \frac{4\pi}{kk'} \chi(-k, -k') \\
= k\epsilon^{-1}(-k, -k')/k',
\]
(3.28)
(3.29)

where
\[
\chi(k, k') = -\frac{k'}{\sqrt{4\pi}} \frac{\partial n_k}{\partial \pi_{k'}}
\]
(3.30)
is the static susceptibility matrix and \(\epsilon^{-1}(k, k')\) is the inverse dielectric matrix. If we make the reasonable assumption that all the eigenvalues of the dielectric matrix are positive, it follows that all the eigenvalues of the matrix of second derivatives of \(E^\pi\) are also positive. The stationary point given by Eq. (3.25) is then a minimum.

Eq. (3.23) is the generalization to inhomogeneous systems of the “subsidiary condition” of Bohm and Pines. It can be rewritten as
\[
\hat{\Omega}_k |\Phi\rangle = 0 \quad (k < k_c),
\]
(3.31)
where
\[
\hat{\Omega}_k = \hat{\pi}_k - \left(\frac{4\pi}{k^2}\right)^{1/2} \langle \hat{n}_k \rangle_0 \hat{1},
\]
(3.32)
and has to be obeyed by \(|\Phi_0\rangle\), the exact ground state of \(\hat{H}_{\text{BP}}\). In the case of a homogeneous system, Eq. (3.31) reduces to \(\hat{\pi}_k |\Phi\rangle = 0\) as derived by Bohm and Pines.

The effect of the subsidiary condition is to reduce the number of degrees of freedom of the extended Hilbert space \(\mathcal{H}_{\text{ext}}\). The reduced Hilbert space satisfying the subsidiary condition is spanned by the set of eigenstates of \(\hat{H}_{\text{BP}}\) of the form \(|\psi\rangle |\pi\rangle\), where
\[
\pi_k = \left(\frac{4\pi}{k^2}\right)^{1/2} \langle \hat{n}_k \rangle_0 \quad \text{for all } k < k_c.
\]
(3.33)
If we have set the parameters \(\pi^0_k\) using Eq. (3.27), the states \(|\psi\rangle\) are then eigenfunctions of the original Hamiltonian, Eq. (3.12). This follows from the definition of the potential \(\hat{V}(r)\), which is such that the Hamiltonian in Eq. (3.22) is the same as the original Hamiltonian of Eq. (3.12) when the value of \(\pi\) is consistent with the subsidiary condition: \(\hat{H}^\pi |\pi_k = \pi^0_k\rangle = \hat{H}\).
The subspace singled out by the subsidiary condition Eq. (3.31) is thus equivalent to the original Hilbert space $\mathcal{H}_R$.

Let us now use the subsidiary condition to evaluate $\Delta E$ and $\Delta V(r)$. For $\Delta E$ we get
\[
\Delta E = \frac{1}{2} \sum_{k<k_c} \frac{4\pi}{k^2} \langle \hat{n}_k \rangle_0 \langle \hat{n}_{-k} \rangle_0 \\
= \frac{1}{2} \int n^l(r)n^l(r')W(r-r')d^3rd^3r',
\] (3.34)
where $n^l(r)$ is the long wavelength ($k < k_c$) part of the ground-state electron density and $W$ is the periodic (Ewald-summed) Coulomb interaction. The constant $\Delta E$ is therefore the long wavelength contribution to the Hartree energy. For $\Delta V$ we get
\[
\Delta V(r) = -\frac{1}{\sqrt{V}} \sum_{k<k_c} \frac{4\pi}{k^2} \langle \hat{n}_k \rangle_0 e^{-ikr},
\] (3.35)
and hence
\[
\nabla^2 [\Delta V(r)] = 4\pi n^l(r).
\] (3.36)
$\Delta V(r)$ is therefore the Hartree potential corresponding to the long wavelength Fourier components of the electronic charge density. Because $\Delta V(r)$ is subtracted from $V(r)$ to give $\tilde{V}(r)$, the extended Hamiltonian $\hat{H}_{BP}$ contains a reduced external potential. The long-range part of the mutual repulsion of the electrons has been absorbed into the plasmon degrees of freedom via the subsidiary condition.

C. The unitary transformation

We have now concluded that we can concentrate on the ground state of the Bohm-Pines Hamiltonian, $\hat{H}_{BP}$, from Eq. (3.21) instead of the ground state of the original Hamiltonian from Eq. (3.12), provided we choose the constants $\pi^0_k$ and hence the effective potential $\tilde{V}$ in accordance with Eq. (3.27). The oscillator-space part of the ground state $|\Phi_0\rangle$ of $\hat{H}_{BP}$ is then equal to $|\pi^0\rangle$, and the real-space part is the physical ground state $|\psi_0\rangle$.

Eq. (3.24) specifies $\pi^0_k$ in terms of the ground-state density, which is obtained by solving $\hat{H}_{BP}$. Unfortunately, this Hamiltonian depends on the parameters $\pi^0_k$ calculated from its
ground state, and so we are faced with a self-consistency problem analogous to those encountered in bandstructure calculations. We could in principle devise an iterative algorithm to home in on a self-consistent solution, but this is unnecessary. We only need the ground-state density, not the wave function itself, and it is known that the LDA gives reasonably good ground-state densities in most solids. In practice, therefore, we can use the LDA density \( \langle \hat{n}_k \rangle_{\text{LDA}} \) to obtain a good approximation for \( \pi_k \):

\[
\pi_k \approx \left( \frac{4\pi}{k^2} \right)^{1/2} \langle \hat{n}_k \rangle_{\text{LDA}} .
\]  

Unsurprisingly, the Bohm-Pines extended Hamiltonian cannot be solved exactly. It may, however, be solved approximately by means of a unitary transformation. We use the unitary operator

\[
\hat{S} = \exp \left[ -i \sum_{k<k_c} \frac{4\pi}{k^2} \hat{q}_k \hat{n}_k \right]
\]

to transform an eigenstate \( |\Phi\rangle \) of \( \hat{H}_{\text{BP}} \) into an eigenstate \( |\Phi^{\text{new}}\rangle = \hat{S}|\Phi\rangle \) of the transformed Hamiltonian \( \hat{H}^{\text{new}}_{\text{BP}} = \hat{S}\hat{H}_{\text{BP}}\hat{S}^\dagger \). (In general, all operators transform according to \( \hat{O}^{\text{new}} = \hat{S}\hat{O}\hat{S}^\dagger \).) The position operators \( \hat{r}_i \) and \( \hat{q}_k \) are unchanged by the transformation because they commute with \( \hat{S} \). The momentum operators transform as follows:

\[
\hat{p}_i \rightarrow \hat{p}_i^{\text{new}} = \hat{p}_i + i \left( \frac{4\pi}{V} \right)^{1/2} \sum_{k<k_c} \hat{q}_k \epsilon_k e^{i\epsilon_k \cdot \hat{r}_i} ,
\]

\[
\hat{n}_k \rightarrow \hat{n}_k^{\text{new}} = \hat{n}_k + \left( \frac{4\pi}{k^2} \right)^{1/2} \hat{n}_k ,
\]

where \( \epsilon_k = \frac{k}{k} \) is a unit vector in the \( k \) direction. The transformations of the momentum operators may be checked using the general expansion,

\[
e^{\hat{\bar{X}}} \hat{O} e^{-\hat{\bar{X}}} = \hat{O} + \frac{1}{2} [\hat{X}, \hat{O}] + \frac{1}{2} \left[ \hat{X}, [\hat{X}, \hat{O}] \right] + \ldots,
\]

with \( \hat{S} = e^{\hat{\bar{X}}} \). When \( \hat{O} \) is one of the momentum operators, \( \hat{n}_k \) or \( \hat{p}_i \), the first commutator \( [\hat{X}, \hat{O}] \) only contains position operators, and so higher order commutators such as \( [\hat{X}, [\hat{X}, \hat{O}]] \) all vanish.
The final result of the unitary transformation defined by Eq. (3.38) is the Hamiltonian:

\[
\hat{H}_{\text{BP}}^{\text{new}} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_{k>k_c} \frac{\hat{n}_k \hat{n}_k^\dagger}{k^2} \\
- \frac{2\pi N}{V} \sum_k \frac{1}{k^2} + \sum_i \hat{V}(\hat{r}_i) \\
+ i \left( \frac{4\pi}{V} \right)^{1/2} \sum_{k<k_c} \sum_i \varepsilon_k \cdot \left( \frac{\hat{p}_i - k}{2} \right) \hat{q}_k e^{i k \cdot \hat{r}_i} \\
+ \frac{2\pi}{\sqrt{V}} \sum_{k,k'<k_c} \left( \varepsilon_k \cdot \varepsilon_{k'} \right) \hat{q}_k \hat{q}_{-k'} \hat{n}_{k+k'} \\
+ \frac{1}{2} \sum_{k<k_c} \hat{n}_k \hat{n}_k - \frac{1}{4} \sum_{k<k_c} \sum_{k<k'} \varepsilon_k \cdot \varepsilon_{k'} \hat{q}_k \hat{q}_{-k} \hat{n}_{k+k'} - \frac{1}{2} \sum_{k<k_c} \hat{n}_k \hat{n}_k 
\] (3.43)

which is obtained by replacing \( \hat{p}_i \) and \( \hat{n}_k \) in Eq. (3.21) by \( \hat{p}_i^{\text{new}} \) and \( \hat{n}_k^{\text{new}} \). The subsidiary condition becomes

\[
\hat{\Omega}_k^{\text{new}} | \Phi^{\text{new}} \rangle = 0 \quad (k < k_c),
\] (3.44)

where

\[
\hat{\Omega}_k^{\text{new}} = \hat{n}_k + \left( \frac{4\pi}{k^2} \right)^{1/2} (\hat{n}_k - \langle \hat{n}_k \rangle_0).
\] (3.45)

We now make the random-phase approximation, which amounts to replacing the \( \hat{n}_{k-k'} = V^{-1/2} \sum_i e^{i(k-k') \cdot \hat{r}_i} \) factor in the fourth line of Eq. (3.43) by its ground-state expectation value. In uniform systems the electronic positions \( \hat{r}_i \) are random and so the phases are also random; the expectation value of \( \hat{n}_{k-k'} \) is therefore equal to \( N\delta_{k,k'}/\sqrt{V} \). In inhomogeneous systems we have to evaluate the expectation value of the (untransformed) operator \( \hat{n}_{k-k'} \) in the transformed ground state \( | \Phi^{\text{new}} \rangle \). Since the density operator \( \hat{n}(\hat{r}) = \sum_i \delta(\hat{r}_i - \hat{r}) \) commutes with the unitary transformation, it follows that

\[
\langle \Phi^{\text{new}} | \hat{n}(\hat{r}) | \Phi^{\text{new}} \rangle = \langle \Phi | \hat{S}^\dagger \hat{n}(\hat{r}) \hat{S} | \Phi \rangle = \langle \Phi | \hat{n}(\hat{r}) | \Phi \rangle.
\] (3.46)

The required expectation value of \( \hat{n}_{k-k'} \) is therefore equal to the Fourier component \( \langle \hat{n}_{k-k'} \rangle_0 \) of the ground-state electron density of the original (untransformed) Bohm-Pines Hamiltonian from Eq. (3.21).
The term on the third line of Eq. (3.43) may be rewritten as

\[
i \left(\frac{4\pi}{V}\right)^{1/2} \sum_{k<k_c} \hat{j}_k \varepsilon_k \cdot \hat{j}_k ,
\]

(3.47)

where \( \hat{j}_k = \sum_i \{ \hat{p}_i, e^{i\mathbf{k} \cdot \mathbf{r}_i} \} \) is the current density operator. Following Bohm and Pines, this plasmon-electron coupling term will be neglected. To justify this approximation (and indeed the RPA) we can appeal to the measured physical properties of interacting electron gases; we know that the plasmons are well defined when \( k < k_c \), and hence that the plasmon-electron coupling terms must indeed be small.

A more physical discussion of the RPA may be found in Appendix A.

D. The RPA ground state

The two approximations described above decouple the electrons and plasmons and reduce the transformed Hamiltonian of Eq. (3.43) to the RPA Hamiltonian \( \hat{H}_\text{RPA} = \hat{H}_\text{sr} + \hat{H}_p \). The first two lines of Eq. (3.43) yield the short-range electronic Hamiltonian,

\[
\hat{H}_\text{sr} = \frac{1}{2} \sum_i \hat{p}_i^2 + 2\pi \sum_{k>k_c} \frac{\hat{n}_k \hat{n}^\dagger_k}{k^2}

- \frac{2\pi N}{V} \sum_k \left( \frac{1}{k^2} + \sum_i \hat{V}(\mathbf{r}_i) \right) ,
\]

(3.48)

and the last two lines yield the plasmon Hamiltonian,

\[
\hat{H}_p = \frac{1}{2}(\hat{\pi} \cdot \hat{\pi}^\dagger + \hat{\mathbf{q}} \cdot M \cdot \hat{\mathbf{q}}^\dagger) ,
\]

(3.49)

where the matrix \( M \) is given by

\[
M_{k,k'} = (\varepsilon_k \cdot \varepsilon_{k'}) \frac{1}{V} \int e^{i(k-k') \cdot \mathbf{r}} \omega_p^2(\mathbf{r}) d^3r ,
\]

(3.50)

and we have introduced a position dependent local plasma frequency defined by \( \omega_p^2(\mathbf{r}) = 4\pi n(\mathbf{r}) \). The full ground state of \( \hat{H}_\text{RPA} \) is the product of the ground states of \( \hat{H}_\text{sr} \) and \( \hat{H}_p \).
1. The plasmon ground state

If we choose to work in a representation in which the \( \hat{\pi}_k \) operators are diagonal, the plasmon ground state takes the standard simple harmonic oscillator form:

\[
\Psi_p \propto \exp \left[ -\frac{1}{2} \sum_{k,k' < k_c} \pi^*_k \left( M^{-1/2} \right)_{k,k'} \pi_{k'} \right].
\]

(3.51)

The matrix \( M^{-1/2} \) is well defined since all the eigenvalues of the Hermitian matrix \( M \) are greater than zero. The fact that the \( \hat{\pi}_k \) and \( \hat{q}_k \) operators are non-Hermitian may cause some confusion here, but one can easily rewrite the \( k \)-space Hamiltonian of Eq. (3.49) in real space using Eqs. (3.17) and (3.18). The real-space operators \( \hat{\pi}(r) \) and \( \hat{q}(r) \) are Hermitian, and so the plasmon Hamiltonian is then a set of coupled Hermitian harmonic oscillators. The ground state of these oscillators is

\[
\Psi_p \propto \exp \left[ -\frac{1}{2} \int \pi(r) M^{-1/2}(r,r') \pi(r') d^3r d^3r' \right],
\]

(3.52)

which reduces to Eq. (3.51) when re-expressed in \( k \)-space.

2. The short-range ground state

If we make use of the expression for \( \tilde{V} \) from Eq. (3.14) and the condition \( \pi^0_k = \sqrt{4\pi/k^2} \langle \hat{n}_k \rangle_0 \) from Eq. (3.27), the short-range Hamiltonian of Eq. (3.48) becomes:

\[
\hat{H}_{sr} = \frac{1}{2} \sum_i \hat{p}_i^2 + \sum_i V(\hat{r}_i)
+ 2\pi \sum_{k > k_c} \frac{\hat{n}_k \hat{n}_k^\dagger}{k^2} - \frac{2\pi N}{V} \sum_k \frac{1}{k^2}
+ \frac{1}{\sqrt{V}} \sum_i \sum_{k < k_c} \frac{4\pi \langle \hat{n}_k \rangle_0}{k^2} e^{-i\hat{k} \cdot \hat{r}_i}
- 2\pi \sum_{k < k_c} \frac{\langle \hat{n}_k \rangle_0 \langle \hat{n}_{-k} \rangle_0}{k^2}.
\]

(3.53)

The first two lines are identical to the original Hamiltonian, Eq. (3.12), but with the small \( k \) (long wavelength) contributions to the electron-electron interactions omitted. The third line is the Hartree potential corresponding to those long wavelength Coulomb interactions,
The short-range Hamiltonian is therefore equivalent to the original Hamiltonian, Eq. (3.12), but with the long wavelength parts of the Coulomb interaction treated within the Hartree approximation. Since the long wavelength parts of the effective potentials used in Hartree-Fock and LDA calculations are both dominated by the Hartree contributions, we might equally well say that \( \hat{H}_{sr} \) is equivalent to the original Hamiltonian but with the small \( k \) Coulomb interactions approximated using Hartree-Fock or LDA, provided the HF or LDA densities are sufficiently similar to the exact ground state density. The short-range Hamiltonian still contains the full Coulomb interaction for \( k > k_c \), and so still diverges like \( 1/r_{ij} \) whenever two electrons approach each other. The electron-electron cusps therefore appear in the short-range electronic wave function, not in the Jastrow factor that describes the plasmons.

In practice, of course, we do not attempt to solve \( \hat{H}_{sr} \) exactly, but treat it within an independent electron approach such as Hartree-Fock or LDA. This additional approximation replaces the short-range part of the electron-electron interaction by a mean field, which simply adds to the long wavelength mean field already introduced by the RPA. The overall effect is equivalent to starting from the original Hamiltonian and replacing the full interaction by a mean field. This implies that one can obtain the short-range “electronic” part of the RPA wave function by starting from the original fully interacting Hamiltonian and treating it using any sensible mean-field approximation. The best single-particle orbitals to use in the Slater determinant are therefore very close to the familiar Hartree-Fock or LDA orbitals; they are not significantly altered by the presence of the RPA Jastrow factor from Eq. (3.61).

One drawback of treating the short-range Hamiltonian within a mean-field approximation is that this neglects the electron-electron cusps that should be present in the short-range electronic wave function. The cusps play an important role in reducing the total energy of the many-electron system, and so the trial wave function may be significantly improved by
building them into the Jastrow factor.

E. Inverting the unitary transformation

The ground state of $\hat{H}_{\text{RPA}}$ is the product of the ground states of $\hat{H}_{\text{sr}}$ and $\hat{H}_{\text{p}}$, neither of which commutes with the transformed subsidiary condition, Eq. (3.44). This implies that, unlike the ground state of $\hat{H}_{\text{BP}}$, the ground state of $\hat{H}_{\text{RPA}}$ need not obey the subsidiary condition automatically. In consequence, the approximate ground state of $\hat{H}_{\text{BP}}$ obtained by applying the back transformation, $\hat{S}^\dagger$, to the ground state of $\hat{H}_{\text{RPA}}$, need not be an eigenfunction of the plasmon momentum operators, and we can no longer extract an approximation to the spatial ground state by simply forgetting about the $|\pi\rangle$ factor in a product wave function of the form $|\psi\rangle|\pi\rangle$. Fortunately, however, the subsidiary condition is still exact (no approximations were made in transforming it), and so still defines the subspace of the extended Hilbert space in which the true ground state lies. We can therefore take the ground state of the approximate Hamiltonian, $\hat{H}_{\text{RPA}}$, and project it onto that subspace. The projection operator may be applied before or after the back transformation, but if we choose to make the back transformation first it is not difficult to see that the required projection operator is

$$\prod_{k<k_c} \left| \pi_k = \pi_k^0 \langle \pi_k = \pi_k^0 | \right.$$ (3.55)

As discussed in Sec. [??D2], we approximate the ground state of $\hat{H}_{\text{sr}}$ as a Slater determinant $D$, and so the approximate ground state of the full Hamiltonian $\hat{H}_{\text{RPA}}$ is $\Phi_{\text{RPA}} \propto \Psi_{\text{p}}D$. We can now obtain an approximate ground state of the original Hamiltonian $\hat{H}_{\text{BP}}$ by back transforming using the inverse of the unitary transformation. The only important effect of the back transformation is to shift the numbers $\pi_k$ appearing in $\Psi_{\text{p}}$ by $-(4\pi/k^2)^{1/2}n_k$:

$$\pi_k \rightarrow \pi_k - \left(4\pi/k^2\right)^{1/2} n_k,$$ (3.56)

where $n_k = V^{-1/2} \sum_i e^{i\mathbf{k} \cdot \mathbf{r}_i}$. This can be verified by observing that, when evaluating a back-
transformed wave function $\Psi^{\text{old}}(\{r_i\}, \{\pi_k\}) = \langle \{r_i\}, \{\pi_k\}|\hat{S}^\dagger|\Psi \rangle$, we can apply the transformation to the bra $\langle \{r_i\}, \{\pi_k\} |$ rather than the ket $|\Psi \rangle$. But since

$$\hat{\pi}_k \hat{S} |\{r_i\}, \{\pi_k\} \rangle = \hat{S} (\hat{\pi}_k - (4\pi/k^2)^{1/2} \hat{n}_k) |\{r_i\}, \{\pi_k\} \rangle$$

$$= \left(\pi_k - (4\pi/k^2)^{1/2} n_k\right) \hat{S} |\{r_i\}, \{\pi_k\} \rangle ,$$

we see that

$$\hat{S} |\{r_i\}, \{\pi_k\} \rangle = |\{r_i\}, \{\pi_k - (4\pi/k^2)^{1/2} n_k\} \rangle .$$

The $\hat{\pi}_k$ eigenvalues of the transformed bra are therefore shifted by $-(4\pi/k^2)^{1/2} n_k$ relative to those of the original bra. As a result, $\Psi^{\text{old}}(\{r_i\}, \{\pi_k\}) = \Psi(\{r_i\}, \{\pi_k - (4\pi/k^2)^{1/2} n_k\})$.

Applying the projection operator given in Eq. (3.55) replaces the remaining $\pi_k$ by $\pi_k^0 = (4\pi/k^2)^{1/2}\langle \hat{n}_k \rangle_0$. (In the homogeneous case this is zero.) All in all, then, the spatial part of the approximation to the ground state is

$$\Psi \propto \Psi_J D = \exp \left[ \frac{1}{2} \sum_{i,j} \tilde{u}(r_i, r_j) \right] D ,$$

where

$$\tilde{u}(r, r') = -4\pi \sum_{k,k'<k_c} \left[ \frac{e^{-ik\cdot r}}{\sqrt{V}} - \frac{\langle \hat{n}_{-k} \rangle_0}{N} \right] \left[ M^{-\frac{1}{2}} \right]_{kk'} \left[ e^{ik'\cdot r - \langle \hat{n}_{k'} \rangle_0} \right]_{kk'} \left[ e^{ik'\cdot r} - \frac{\langle \hat{n}_{k'} \rangle_0}{N} \right] .$$

(3.60)

The RPA Jastrow factor includes constant terms, one-electron terms, and two-electron terms. The constant terms may be ignored as they only affect the normalization of the wave function. The remaining one- and two-electron terms may then be disentangled and the Jastrow factor rewritten in the form,

$$\Psi_J \propto \exp \left[ \frac{1}{2} \sum_{i,j} u(r_i, r_j) + \sum_i \chi(r_i) \right] ,$$

(3.61)
where \( u(\mathbf{r}, \mathbf{r}') \) and \( \chi(\mathbf{r}) \) are defined via:

\[
u(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{k, k'<k_c} e^{-i k \cdot \mathbf{r}} \frac{4 \pi [M^{-1/2}]}{k k'} e^{i k' \cdot \mathbf{r}'},
\]

and

\[
\chi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{k, k'<k_c} e^{-i k \cdot \mathbf{r}} \frac{4 \pi [M^{-1/2}]}{k k'} \langle \hat{n}_k \rangle_0.
\]

where, as in Eq. (3.34), \( n^l(\mathbf{r}) \) is the long wavelength \( k < k_c \) part of the ground-state electron density. The derivation of Eq. (3.63) made use of the symmetry \( M_{k, k'} = M_{-k', -k} \), which follows from Eq. (3.50). In \( k \)-space, the relationship between \( u \) and \( \chi \) takes the form,

\[
\chi(k) = -\sum_{k'<k_c} u(k, k') n(k') ,
\]

discussed in Sec. II C.

In a homogeneous system, Eq. (3.50) states that \( M_{k, k'} = \omega_p^2 \delta_{k, k'} \). The \( \chi \) function therefore vanishes and the \( u \) function becomes

\[
u^\text{hom}(k, k') = -\frac{4 \pi}{\omega_p} \frac{1}{k k'} \delta_{k, k'} .
\]

Transforming to real space we obtain

\[
\nu^\text{hom}(\mathbf{r}, \mathbf{r}') = \nu^\text{hom}(|\mathbf{r} - \mathbf{r}'|) = -\frac{1}{\omega_p} \sum_{k, k'<k_c} e^{-i k \cdot \mathbf{r} + i k' \cdot \mathbf{r}'} \frac{4 \pi}{k k'} \delta_{k, k'} = -\frac{1}{\omega_p} \sum_{k<k_c} e^{-i k \cdot (\mathbf{r} - \mathbf{r}')} \frac{4 \pi}{k^2} .
\]

If \( k_c \) is set equal to infinity this gives

\[
\nu^\text{hom}(|\mathbf{r} - \mathbf{r}'|) = -\frac{1}{\omega_p |\mathbf{r} - \mathbf{r}'|} .
\]

For finite \( k_c \), the divergence of \( u(|\mathbf{r} - \mathbf{r}'|) \) at small \( |\mathbf{r} - \mathbf{r}'| \) is suppressed, but the \( 1/|\mathbf{r} - \mathbf{r}'| \) decay at large \( |\mathbf{r} - \mathbf{r}'| \) remains more or less unaltered.
F. The cusp conditions in inhomogeneous systems

Section II B explained how cusps may be built into a homogeneous RPA Jastrow factor by adding an exponential factor to the \( u \) function:

\[
u(r) = -\frac{1}{\omega_p r} \left(1 - e^{-r/F}\right).
\] (3.69)

At large \( r \) this \( u \) function has the \( 1/(\omega_p r) \) behavior implied by the RPA, while at small \( r \) it tends smoothly towards the required cusp at \( r = 0 \). When supplemented by appropriate \( \chi \) functions, such Jastrow factors are remarkably successful. It is therefore worth considering how we might add cusps to our inhomogeneous RPA \( u \) function.

This is not easy, since the inhomogeneous \( u \) function is given as a complicated truncated double Fourier series. The series determines the behavior of \( u(r, r') \) when \( r - r' \) is large, and we have to find a way of splicing this known long-range behavior onto the cusp at small \( r - r' \). The cusp fixes the slope of \( u(r, r') \) as \( |r - r'| \to 0 \), but does not determine its position-dependent value at the point \( r = r' \). This makes it difficult to implement simple interpolation schemes that use different functions to describe \( u \) at small and large \( r - r' \).

The introduction of a multiplicative factor, as in the homogeneous \( u \) function of Eq. (3.69), is equally problematic.

It turns out that this interpolation problem is easiest to handle when expressed in \( k \)-space. This might seem unlikely at first, since a true cusp can only be generated by a computationally intractable infinite Fourier sum. In practice, however, it appears that satisfactory approximate cusps can be introduced using Fourier sums with manageable numbers of terms. The \( k \)-space cutoff needs to be large enough to ensure that the real space volume within which the cusp is not represented correctly is small, and hence that the resulting errors contribute little or nothing to expectation values.

Eq. (3.69) can be Fourier analyzed to give:

\[
u(k) = \frac{-4\pi}{\sqrt{V\omega_p}} \frac{1/F^2}{k^2 + 1/F^2}.
\] (3.70)
Eqs. (2.13) and (2.14) show that $1/F^2 = C_\omega p$, where $C = 1$ for antiparallel spins and $C = 1/2$ for parallel spins. Hence

$$u(k) = \frac{-4\pi C}{\sqrt{V} k^2 (k^2 + C_\omega p)}.$$  

(3.71)

In section IV B we test a homogeneous $u$ function defined using a truncated Fourier series of this form, and find that most of the cusp energy can be retrieved using a reasonably low cutoff.

Eq. (3.71) defines a natural $k$-space crossover, $k_x$, given by $k_x^2 = C_\omega p$. The terms with $k < k_x$ produce the RPA behavior at large $r$, while for $k > k_x$ we have $u(k) \propto 1/k^4$, which generates the cusp. The density dependence of $k_x$ differs from that of the plasmon cutoff $k_c$ from Eq. (3.3). It turns out, however, that for typical metallic densities $k_c$ and $k_x$ are both of the order of $k_F$. The $k^2 + C_\omega p$ factor in the denominator of Eq. (3.71) therefore allows us to introduce the cusp without significantly affecting the large $r$ ($k < k_c$) behavior implied by the RPA. If the density is extremely small, $k_x \propto \omega_p^{1/2} \propto n^{1/4}$, is smaller than $k_c \propto n^{1/6}$, and so the $k$-space method of imposing the cusp is no longer consistent with the RPA limit we expect when $k < k_c$.

Equation (3.71) suggests a simple $k$-space prescription for building a cusp into the inhomogeneous Jastrow factor. We write the inhomogeneous Jastrow factor as a double Fourier series,

$$u(r, r') = \frac{1}{V} \sum_{k, k'} e^{-ikr} u(k, k') e^{ik'r'},$$  

(3.72)

noting that in a homogeneous system we have $u(k, k') = \sqrt{V} u(k) \delta_{k,k'}$. We use this relationship to rewrite the homogeneous $u$ function of Eq. (3.71) in a form suitable for generalization to the inhomogeneous case,

$$u(k, k') = \frac{4\pi C}{kk'} (kk' \delta_{k,k'} + C_\omega p \delta_{k,k'})^{-1},$$  

(3.73)

interpreting the inversion as that of a (diagonal) matrix. In the absence of cusps, we have seen that the homogeneous Jastrow factor may be obtained from the inhomogeneous one by replacing
by \( \omega_p^2 \delta_{k,k'} \). As we now wish to extrapolate from a homogeneous Jastrow factor to an inhomogeneous one, we do the opposite and replace \( \omega_p^2 \delta_{k,k'} = (\omega_p^2 \delta_{k,k'})^{1/2} \) by the matrix square root \( M_{k,k'}^{1/2} \). Eq. (3.73) then becomes

\[
\begin{align*}
M_{k,k'} &= \frac{1}{V} \frac{(k \cdot k')}{kk'} \int e^{i(k-k') \cdot r} \omega_p^2(r) d^3r \\
&= \frac{4\pi C}{kk'} \left( \delta_{k,k'} + C M_{k,k'}^{1/2} \right)^{-1} \\
&= \frac{4\pi C}{kk'} \left( \delta_{k,k'} + \frac{CM_{k,k'}^{1/2}}{kk'} \right)^{-1}.
\end{align*}
\] (3.74)

The matrix to be inverted is no longer diagonal, but remains Hermitian and positive definite.

If we make the reasonable assumption that the Fourier series for \( \omega_p^2(r) \) converges fairly rapidly, the elements of the matrix \( M \) are constant along the diagonal and fall off as we move away from the diagonal. For large \( k \) and \( k' \), this guarantees that \( u(k,k') \) is dominated by the \( 1/(kk')^2 \approx 1/k^4 \) prefactor, generating a cusp. For small \( k \) and \( k' \) we have

\[
u(k,k') \approx -\frac{4\pi C}{kk'} \left( CM_{k,k'}^{1/2} \right)^{-1} = -4\pi \frac{M_{k,k'}^{-1/2}}{kk'},
\] (3.76)

which is the RPA result.

The \( u \) function of Eq. (3.75) therefore interpolates smoothly between the anisotropic long-range correlation term derived from the inhomogeneous RPA and the cusp at short range. In \( k \)-space we now have a continuous crossover from collective behavior to two-particle scattering instead of a sudden and rather unphysical cutoff at \( k_c \).

G. The one-body term

The introduction of the cusp modifies the \( k < k_c \) Fourier components of the RPA \( u \) function and introduces nonzero Fourier components with \( k > k_c \). In addition, it makes the \( u \) function spin dependent, suggesting that we need a spin-dependent one-body term. We therefore generalize our expression for \( \chi(k) \) from Eq. (3.65) by extending the wave vector sum to include components with \( k > k_c \) and introducing a sum over spin indices,
\[ \chi_{\uparrow}(k) = -\sum_{k'} [u_{\uparrow\uparrow}(k, k') n_{\uparrow}(k') + u_{\uparrow\downarrow}(k, k') n_{\downarrow}(k')] , \] (3.77)

with an equivalent formula for \( \chi_{\downarrow}(k) \). In a spin-unpolarized system, where \( n_{\uparrow}(k') = n_{\downarrow}(k') = \frac{1}{2} n(k') \), this reduces to

\[ \chi_{\uparrow}(k) = -\sum_{k'} \frac{1}{2} [u_{\uparrow\uparrow}(k, k') + u_{\uparrow\downarrow}(k, k')] n(k') . \] (3.78)

In the case of a homogeneous correlation term \( u \) this further reduces to

\[ \chi_{\uparrow}(k) = -\frac{1}{2} \sqrt{V} [u_{\uparrow\uparrow}(k) + u_{\uparrow\downarrow}(k)] n(k) , \] (3.79)

as first proposed by Malatesta et al.\[12\].

**IV. RESULTS**

This section assesses the effectiveness and accuracy of QMC trial wave functions containing RPA Jastrow factors. Section IV A describes the systems studied and explains how the results are presented; Sec. IV B considers homogeneous systems; and Sec. IV C looks at inhomogeneous systems.

All the results were obtained using trial wave functions of the standard Slater-Jastrow form, where the spin-up and spin-down Slater determinants were constructed using accurate LDA orbitals. The Jastrow factor contained two- and one-body terms, \( u(r_i, r_j) \) and \( \chi(r_i) \), of various different types. Note that from now on we drop the \( u(r_i, r_i) \) self-interaction terms from the Jastrow factor. This is equivalent to altering \( \chi(r_i) \) by a negligible amount (ca. 5%).

The energy averages discussed in the rest of this section were all accumulated using samples of 10000 statistically independent configurations of all the electrons; the quoted errors are standard deviations of the mean of the local energy.

**A. System geometry**

In one-electron bandstructure calculations the energy eigenfunctions \( \psi_k(r) \) may be obtained by solving the one-electron Schrödinger equation within a single unit cell subject
to Bloch boundary conditions. Properties of the infinite crystal may then be obtained by evaluating Brillouin zone integrals (i.e. averaging over boundary conditions). In QMC calculations, however, we have to take account of all the electrons simultaneously, and it is no longer possible to reduce the problem to a single unit cell. Instead, we consider a model solid consisting of a finite simulation subject to periodic (not Bloch) boundary conditions. The simulation cell is made as large as possible to minimize the finite-size errors, and normally consists of several primitive unit cells containing a few hundred electrons in total.

The simulation cell we choose is the Wigner-Seitz cell of a face-centered cubic (FCC) lattice. Since we use periodic boundary conditions, any electron that moves out through one face of this cell immediately re-enters through the opposite face. The simulation-cell Hamiltonian obeys the same periodic boundary conditions, and hence a periodic model potential energy is required; we use the potential energy per cell of an infinite lattice of identical copies of the simulation cell. Since the Wigner-Seitz cell of an FCC lattice is close to spherical, the interactions between electrons in neighboring copies of the simulation cell are smaller than for most other geometries, which helps to reduce the finite-size errors. It is important not to confuse the simulation-cell lattice with the actual lattice structure of the solid; the simulation cell may contain many primitive unit cells, and these need not be face-centred cubic. The lattice vectors of the FCC simulation-cell lattice will be denoted by $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$, and the corresponding body-centered cubic (BCC) reciprocal lattice vectors by $\mathbf{B}_1$, $\mathbf{B}_2$, and $\mathbf{B}_3$.

For reasons of computational efficiency, we have chosen to study electron gas systems subject to external potentials that vary along the $\mathbf{B}_3$ direction only,

$$V_{\text{ext}}(\mathbf{r}) = V_0 \cos(\mathbf{B}_3 \cdot \mathbf{r}), \quad (4.1)$$

where $V_0 = 1$ in atomic units. Since $\mathbf{B}_3$ is a reciprocal lattice vector, this choice ensures that the potential has the same periodicity as the simulation cell. The electron density and $\chi$ functions, which also vary only in the $\mathbf{B}_3$ direction, share this periodicity.

The one- and two-body terms must also respect the periodic boundary conditions applied
to the simulation cell. This implies that analytic Jastrow factors based on the $u$ function of Eq. (3.69) must be made periodic by including contributions from all the electrons in a periodic lattice of identical copies of the simulation cell. Since the analytic $u$ function decays like $1/r$ at large $r$, the sum of contributions is evaluated using Ewald summation techniques. Numerical Jastrow factors calculated from the inhomogeneous RPA are periodic by construction.

The next two subsections contain a number of figures showing electron densities, $\chi$ functions, and $u$ functions. Charge densities and $\chi$ functions are plotted along the $B_3$ direction from one side of the simulation cell to the other. The inhomogeneous two-body term $u(r_1,r_2)$ is more difficult to represent. We have chosen to fix the position $r_1$ of the first electron, while sweeping $r_2$ along the $B_3$ direction on a line passing through $r_1$. Figure 1 shows the three positions of the first electron considered. Note that because $A_3$ and $B_3$ are not the same, moving along a line parallel to $B_3$ does not bring you back to a point equivalent to (i.e. differing by a lattice vector from) the starting point until you have passed through three layers of simulation cells. This means that although $u(r_1,r_2)$ always has the full periodicity of the simulation cell, this is not always apparent from the plots. Note also that all Jastrow factors are symmetric on interchange of $r_1$ and $r_2$.

**B. Homogeneous systems**

The FCC simulation cell considered in this section held a uniform electron gas of 61 up-spin electrons and 61 down-spin electrons, giving 122 electrons in total. The density parameter $r_s$ was equal to 2, corresponding to a Fermi wave vector $k_F=0.96a_0^{-1}$. Two different Jastrow factors were considered:

*a. Homogeneous RPA without cusps.* The homogeneous RPA theory suggests using a correlation term of the form,

$$u(r_i, r_j) = -\frac{4\pi}{V\omega_p} \sum_{k<k_c} \frac{1}{k^2} e^{i\mathbf{k} \cdot (r_i - r_j)}.$$  (4.2)
We saw in Sec. III A that for typical metallic densities the cutoff $k_c$ is set to a value comparable to the Fermi wave vector $k_F$.

b. Homogeneous RPA with cusps. In Sec. III B we saw how a cusp may be introduced by adding an exponential factor to the $k_c \to \infty$ limit of the homogeneous RPA $u$ function,

$$u_{\sigma_i \sigma_j}(r_{ij}) = -\frac{1}{\omega_p r_{ij}}(1 - e^{-r_{ij}/F_{\sigma_i \sigma_j}}), \quad (4.3)$$

where $F_{\sigma_i \sigma_j}$ is chosen appropriately.

Table I shows the local energy averages and standard deviations obtained in VQMC simulations using these two Jastrow factors. For comparison, we also show results obtained using a “Hartree-Fock” trial function including up- and down-spin Slater determinants of LDA orbitals (in this case plane waves) but no Jastrow factor. The introduction of an RPA Jastrow factor without a cusp lowers the calculated energy considerably but has little effect on the standard deviation. The introduction of the cusp lowers the energy greatly and also reduces the standard deviation. It is clear that the presence of the cusp is vital if accurate total energies are to be obtained.

The cuspless RPA results shown in Table I were obtained using a value of $k_c$ equal to the Fermi wave vector $k_F$, but we also investigated the limit as $k_c$ tends to infinity, in which case $u(r_{ij}) \to -1/(\omega_p r_{ij})$. Since we know that the description of screening in terms of collective plasmon modes is invalid at short distances, it was no surprise that this limiting form gave very poor results. The residual two-electron interactions in the short-range Hamiltonian lead to a cusp-like behavior in the wave function at close distances, not a $-1/(\omega_p r_{ij})$ divergence.

In Sec. III F we saw how the $u$ function with a cusp from Eq. (4.3) may be represented as a Fourier series,

$$u(k) = \frac{-4\pi}{\sqrt{V}} \frac{C}{k^2(k^2 + C\omega_p)}, \quad (4.4)$$

where $C = 1$ for antiparallel spins and $C = 1/2$ for parallel spins. We can investigate the usefulness of this representation by cutting off the series at a wave vector $k_n$ and varying $k_n$ to see how fast the calculated VQMC energy approaches the $k_n \to \infty$ limit. The hope is that
with a reasonably small $k$-space cutoff we will be able to produce a Jastrow factor that gives essentially the $k_n \to \infty$ energy. Figure 2 shows the convergence of the energy graphically. It can be seen that a cutoff of $k_n = 3.95a_0^{-1}$ produces a wave function with the same energy (to within statistical uncertainties) as an infinite cutoff. The $3.95a_0^{-1}$ cutoff is small enough to be computationally feasible, and so there is no difficulty in representing the cusp in $k$-space. Note also how the standard deviation tends to zero as the energy improves.

C. Inhomogeneous systems

As mentioned above, the inhomogeneous systems we consider have a background potential that varies in one dimension only. The LDA electron density of the unpolarized 64 electron simulation cell considered in this subsection is shown in Fig. 3. This system is strongly inhomogeneous (for comparison, a typical interatomic distance in a solid is $\sim 6a_0$; this is roughly the distance between the trough and the peak of the charge density). The average electron density is the same as that of a uniform system with $r_s = 2$ and Fermi wave vector $k_F = 0.96a_0^{-1}$.

In addition to investigating the influence of the cusp, as in the homogeneous case, we must also now investigate the effects of the one-body $\chi$ function and compare the accuracies of homogeneous and inhomogeneous $u$ functions. We therefore split this section into three subsections:

1. First we look at the pure (i.e. cuspless) homogeneous RPA Jastrow factor (which has no $\chi$ function) and compare it with the pure inhomogeneous RPA Jastrow factor (which does have a $\chi$ function).

2. Second we investigate the effects of adding cusps to these two correlation factors.

3. Finally we add an ad-hoc one-body $\chi$ term to the homogeneous RPA Jastrow factor.
1. Inhomogeneous RPA without cusps

The inhomogeneous RPA Jastrow factor considered here is the one derived in Sec. IIII (Eqs. (3.61), (3.62), and (3.63)), which includes both $u$ and $\chi$ functions. As always in this work, the matrix $M$ is constructed using the LDA density, and the Slater determinants contain LDA orbitals. The homogeneous Jastrow factor includes the $u$ function from Eq. (4.2) but no $\chi$. In both cases the cutoff $k_c$ is set equal to the Fermi wave vector, $k_0^F=0.96a_0^{-1}$, of a homogeneous system with the same average electron density as the inhomogeneous system.

Table I compares the VQMC energies and standard deviations calculated using the homogeneous and inhomogeneous Jastrow factors. It is clear that the inhomogeneous Jastrow factor is much the better of the two. The reason is apparent from Fig. 3, which demonstrates that the inhomogeneous Jastrow factor, which has a built-in one-body term, produces a near optimal density. Figure 3 also shows that the homogeneous RPA Jastrow factor (which has no one-body term) gives a very poor electron density. This explains why the corresponding VQMC energy is so poor.

In Fig. 4 we plot the inhomogeneous RPA two-body term. Both inhomogeneity and anisotropy can be seen. To aid understanding, Fig. 5 shows the Jastrow factors of three different homogeneous systems, the constant densities of which correspond to the local densities at the central positions of plots A, B, and C, respectively. It is clear that the three inhomogeneous $u$ functions shown in Fig. 4 are much more similar than the three homogeneous $u$ functions shown in Fig. 5. This shows that the inhomogeneous RPA $u$ function is not well approximated by a local-density-like approximation based on the homogeneous RPA. In the low density region (position C), in particular, we find that the inhomogeneous Jastrow factor in Fig. 4 is suppressed relative to the “local density” version of Fig. 5.

At point B, the charge density around the electron is asymmetric, and this is reflected in the anisotropy of the $u$ function. The anisotropy is such that the $u$ function is stronger on the side where the density is lower; this is consistent with the idea that the RPA screening is more effective where the electron density is high.
In summary, we find that the Jastrow factor has a larger range in the low density regions than in the high density regions, consistent with the “local density” picture of Fig. 4 and with the physical expectation that screening should be more effective at high densities. This interpretation also explains the sign of the anisotropy: the $u$ function is weaker on the high density side where the screening is more effective. We find, however, that the range of variation of the inhomogeneous Jastrow factor is much smaller than predicted by the “local density” picture. This suggests that a homogeneous Jastrow factor defined by the averaged density of the underlying inhomogeneous system may not be such a bad approximation.

2. Inhomogeneous RPA with cusps

A cusp may be added to the inhomogeneous RPA $u$ function using the Fourier-space method explained in Sec. III F. The results below are obtained with a Fourier cutoff $k_n$ of $4.95a_0^{-1}$; Fig. 2 suggests that this is large enough to represent the cusp accurately. Since we choose not to change the relationship between the $u$ and $\chi$ functions, Eq. (2.13), the introduction of the cusp also modifies the one-body $\chi$ function.

The addition of the cusp to the inhomogeneous RPA Jastrow factor reduces the calculated VQMC energy from $-13.32(4) \times 10^{-2}$ eV per electron to $-15.81(1) \times 10^{-2}$ eV per electron. This is the best variational estimate of the energy we were able to obtain using any of the Jastrow factors considered in this paper. The addition of cusps to the homogeneous $u$ function does not introduce a one-body term and so the density obtained using the homogeneous RPA Jastrow factor is still poor. Energies calculated using the homogeneous RPA Jastrow factor therefore remain much worse than energies calculated using the inhomogeneous RPA Jastrow factor.

Figure 6, which is analogous to Fig. 4, shows the inhomogeneous RPA $u$ function after the cusp has been added. It is clear that the addition of the cusp greatly reduces the amount of inhomogeneity and anisotropy. Despite the fact that the system is strongly inhomogeneous, the cusp acts as such a stringent constraint that $u(\mathbf{r}_i, \mathbf{r}_j)$ is close to homogeneous. Although
the inhomogeneity derived from the RPA must persist when |ri − rj| is large enough, the
crossover length, 2π/kx, corresponding to the average density r_s=2, is comparable to our
system size. This implies that the form of the u function is largely determined by the cusp
throughout our system. If we had studied larger systems we would have seen the RPA
reassert itself at large |ri − rj|, but previous work on numerical trial function optimization
and finite-size errors has shown that the behavior of the u function at such large values of
|r_i − r_j| has very little effect on the total energy. The fact that the inhomogeneous u function
becomes so homogeneous once the cusp has been added may explain the surprisingly good
performance of the homogeneous u functions used in most QMC simulations of solids.

3. Other one-body terms

In this subsection we compare the quality of analytic one-body terms based on Eq. (2.15)
and numerical one-body terms obtained using variance optimization.

We have already explained that we always construct the χ function appearing in the
inhomogeneous RPA Jastrow factor from the u function and density according to Eq. (2.15).
Although Eq. (2.15) was derived within the RPA, we assume that it holds unaltered even
after the spin-dependent cusps have been added to u. This assumption proves very successful
in practice, yielding χ functions that are not significantly worse than those computed (at
much greater cost) using numerical variance optimization.

When adding a χ function to the homogeneous u function of Eq. (4.3) we have two
options: we could try using Eq. (2.15) again, or we could use variance minimization. Since
u is now a function of |ri − r_j| only, Eq. (2.15) reduces to Eq. (2.16), which was first derived
by Malatesta et al. The impressive accuracy of Eq. (2.16) is shown in Fig. 7, where
we compare the analytic χ function with one obtained using additional numerical variance
optimization. We see that the two χ functions (and hence the two electron densities) are
very similar. Table III shows that the difference between the two VQMC energies is smaller
than the statistical noise in our simulations.
Table IV shows that the inhomogeneous RPA (including the $\chi$ function from Eq. (2.15) and an approximate Fourier representation of the cusp) yields marginally better results than the homogeneous RPA (including the $\chi$ function from Eq. (2.16) and an approximate Fourier representation of the cusp). Comparing these results to the Ewald (i.e. $k_n \rightarrow \infty$) results from Table III, we see that including the exact cusp reduces the variance but has only a negligible effect on the energy. The inhomogeneous numerical Jastrow factor yields a slightly better energy than the Ewald Jastrow factor. The improvement is barely statistically significant, but suggests that the inhomogeneity of the RPA correlations does produce a slight improvement.

V. CONCLUSIONS

Our aim was to better understand the physics underlying the Jastrow factors used in QMC simulations of solids, and to derive improved Jastrow factors for strongly inhomogeneous systems. We began by reviewing Bohm and Pines’ RPA treatment of the homogeneous electron gas and generalizing it to the inhomogeneous case. The result of this analysis was a Slater-Jastrow trial wave function containing an anisotropic inhomogeneous Jastrow factor expressed as a double Fourier sum. The optimal orbitals appearing in the Slater determinants were shown to be close to Hartree-Fock or LDA orbitals, even though these theories do not include Jastrow factors.

The RPA describes the long-range electronic correlations accurately, but not the scattering-like correlations at short distances. We saw, however, that the correct short-range behavior determined by the cusp conditions may easily be imposed on any Jastrow factor represented in $k$-space. When the inhomogeneous RPA result is modified in this way, the result is a parameter-free Jastrow factor with the correct short and long-range behavior.

For systems of a few hundred electrons and an external potential varying in one dimension only, we showed that trial functions incorporating modified RPA Jastrow factors are both accurate and computationally tractable. Since such Jastrow factors are parameter-free,
the time-consuming variance minimization procedure normally used to generate accurate \( \chi \) functions is not required. Surprisingly, however, the inhomogeneity of the two-body \( u \) function yields little benefit in the system we studied, producing an energy only two standard deviations (a barely statistically significant amount) below the best result obtained using a homogeneous \( u \) function. Provided we have a cusp describing the short-range interaction and a one-body term to mend the density, the detailed form of the \( u \) function is not very important. The reason is that the imposition of the cusp conditions, which fixes the gradient of \( u(\mathbf{r}_i, \mathbf{r}_j) \) when \( |\mathbf{r}_i - \mathbf{r}_j| \to 0 \), washes out most of the inhomogeneity of the RPA \( u \) function when \( |\mathbf{r}_i - \mathbf{r}_j| \) is small. It is the short-range correlations that have most effect on the energy, and so the long-range inhomogeneities that remain after the cusp conditions have been imposed have little effect.

If we compare the plasmon cutoff \( k_c (\propto n^{1/6}) \) from Eq. (3.3) with the wave vector \( k_x (\propto n^{1/4}) \) that characterizes the crossover from screening behavior to cusp-like behavior (see Sec. III F), we see that the cusp is relatively less important in high density systems. This suggests that the inhomogeneity of the RPA \( u \) function may produce a more obvious improvement when the average electron density is both large and strongly varying. This is intuitively sensible, since in low density systems we expect the short-range electron-electron scattering described by the cusp to dominate, whereas at higher densities screening and collective effects should be more important. Possible candidates for high density systems include calculations explicitly involving the core electrons, where it is already known that the use of inhomogeneous \( u \) functions is advantageous.\(^2\) Other systems where one might expect inhomogeneities in the correlation term to become important are rare earth elements, where some of the valence electrons are strongly bound to the core.

In summary, we hope that this paper has contributed a better and more general understanding of the physics underlying the Slater-Jastrow trial functions used in most QMC simulations of solids.
APPENDIX A: PHYSICAL INTERPRETATION OF THE RANDOM-PHASE APPROXIMATION

In this appendix we look at the physical interpretation of the Bohm-Pines Hamiltonian \( \hat{H}_{BP}^{new} \) after the application of the unitary transformation discussed in Sec. III C. As expressed in Eq. (3.43) this Hamiltonian appears very complicated. However, if we define a field

\[
\hat{A}(\mathbf{r}) = \left(\frac{4\pi}{V}\right)^{\frac{1}{2}} \sum_{k < k_c} i \hat{q}_k \varepsilon_k e^{i k \cdot \mathbf{r}}
\]  
(A1)

and then calculate \( \hat{E}(\mathbf{r}) = -\frac{d}{dt} \hat{A}(\mathbf{r}) = -i [\hat{H}_{BP}^{new}, \hat{A}(\mathbf{r})] \), we obtain:

\[
\hat{E}(\mathbf{r}) = - \left(\frac{4\pi}{V}\right)^{\frac{1}{2}} \sum_{k < k_c} i \hat{\pi}_{-k} \varepsilon_k e^{i k \cdot \mathbf{r}}.
\]  
(A2)

The transformed Bohm-Pines Hamiltonian may then be written in the much simpler form:

\[
\hat{H}_{BP}^{new} = \frac{1}{2} \sum_i \left[ \hat{p}_i + \hat{A}(\hat{r}_i) \right]^2 - \frac{2\pi N}{V} \sum_k \frac{1}{k^2} \\
+ \frac{1}{8\pi} \int_V \left[ \hat{E}(\mathbf{r}) \right]^2 d^3r + \sum_i \tilde{V}(\hat{r}_i).
\]  
(A3)

The Hamiltonian of Eq. (A3) describes a set of quantum mechanical particles moving in a reduced external potential potential \( \tilde{V}(\mathbf{r}) \) and interacting with a quantum mechanical longitudinal electromagnetic field \( \hat{A}(\mathbf{r}) \). The kinetic energy of the field is associated with the energy density of the electric field in the usual way. The interactions between the particles and the field are also described via the standard coupling to the momentum operators.

The physical interpretation of the transformed subsidiary condition, \( \hat{\Omega}_{k}^{new} | \Phi_{new}^{new} \rangle = 0 \), where \( \hat{\Omega}_{k}^{new} \) is as given in Eq. (3.45), also becomes much clearer when re-expressed in terms of the new fields; it simply sets the Fourier components of

\[
\hat{\Omega}(\mathbf{r}) \propto \text{div} \hat{E}(\mathbf{r}) - 4\pi [\hat{n}(\mathbf{r}) - n(\mathbf{r})]
\]  
(A4)

to zero. The subsidiary condition thus ensures that the electric field is related to the density of the particles via Gauss’s law. Crucially, we found that this constraint is automatically satisfied in the ground state, provided the \( \pi^0 \) have been chosen correctly.
The RPA decouples the electronic and field variables by neglecting the \( \mathbf{p} \cdot \hat{\mathbf{A}} \) terms and treating the quadratic \( \hat{\mathbf{A}}^2 \) terms only approximately by averaging the electron positions. The field part of the decoupled Hamiltonian is then harmonic:

\[
\frac{1}{2} \int_V [\hat{\mathbf{A}}(\mathbf{r})]^2 n(\mathbf{r}) d^3r + \frac{1}{8\pi} \int_V [\hat{\mathbf{E}}(\mathbf{r})]^2 d^3r . \tag{A5}
\]

The resulting wave function no longer obeys Gauss’s law automatically, but a projection operator can be applied to produce a wave function that does.

Eq. (A5) looks disconcertingly simple: it appears that we have three independent harmonic oscillators at every point \( \mathbf{r} \) (one each for the x, y and z components of the vector potential). The apparent simplicity is misleading, however, since the condition that the fields be longitudinal, \( \text{curl} \mathbf{A} = 0 \), couples the oscillators at different points in space and reduces the number of degrees of freedom at any point from three to effectively just one. Dropping this condition and retaining only one scalar oscillator is equivalent to dropping the \( \varepsilon_k \cdot \varepsilon_{k'} \) term in Eq. (3.50) and leads to a local-density-like version of the RPA.
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FIG. 1. In figures showing two-body terms, plots labeled A show $u(\mathbf{r}_1, \mathbf{r}_2)$ as a function of $\mathbf{r}_2$ for $\mathbf{r}_1$ fixed at the peak of the electron density; plots labeled B show $u(\mathbf{r}_1, \mathbf{r}_2)$ for $\mathbf{r}_1$ fixed at the average of the electron density; and plots labeled C show $u(\mathbf{r}_1, \mathbf{r}_2)$ for $\mathbf{r}_1$ fixed at the minimum of the electron density. In all cases, $\mathbf{r}_2$ is swept along the $\mathbf{B}_3$ direction on a line passing through $\mathbf{r}_1$. The relative coordinate $z$ measures the distance between the two electrons and thus equals zero when the two electrons are at the same place, irrespective of the fixed position of $\mathbf{r}_1$.

FIG. 2. The convergence of the VQMC energy as a function of the cutoff $k_n$ used in the truncated Fourier series representation of the $u$ function from Eq. (4.3). The results are for the uniform system considered in Sec. [IV.B], for which $k_F = 0.96a_0^{-1}$. The dotted line shows the calculated value of the energy when $k_n=\infty$ (the standard deviation of this result is too small to show here).
FIG. 3. The electron density of the strongly inhomogeneous 64 electron system considered in Sec. IV C. The LDA density (solid line) is compared to the densities obtained using the homogeneous RPA (dotted line) and the inhomogeneous RPA (dashed line); the $z$-axis lies along the $\mathbf{B}_3$ direction.

FIG. 4. The inhomogeneous RPA $u$ function with no cusp for three different positions of the fixed electron. The results are for the inhomogeneous system considered in Sec. IV C. The definition of $z$ and the positions of A, B, and C are explained in Fig. 1. The Jastrow factor is stronger in the low density region.
FIG. 5. The RPA $u$ functions for three different uniform electron gases, the densities of which are equal to the densities at points A, B, and C of the strongly inhomogeneous 64 electron system considered in Sec. IV C. The definition of $z$ and the positions of A, B, and C are explained in Fig. 1. The homogeneous $u$ functions are of course isotropic.

FIG. 6. The inhomogeneous RPA $u$ function with a cusp for three different positions of the fixed electron. The results are for the strongly inhomogeneous 64 electron system considered in Sec. IV C. The definition of $z$ and the positions of A, B, and C are explained in Fig. 1. The addition of the cusp has much reduced the inhomogeneity and anisotropy observed in Fig. 4.
FIG. 7. Comparison of the $\chi$ function (solid line) obtained from Eq. (2.16) with one (dashed line) obtained using an additional variance minimization. The results are for the strongly inhomogeneous 64 electron system considered in Sec. IV C, using the homogeneous Ewald-summed Jastrow factor with cusp. The corresponding energies, shown in Table II, are equal to within the statistical error.
TABLE I. VQMC local energy averages and standard deviations of the uniform system considered in Sec. [IVB]. Results for three different trial wave functions are shown. The HF trial function has no Jastrow factor. The RPA results use the “pure” RPA $u$ function from Eq. (4.2). The best energies are obtained using the RPA $u$ function with a cusp from Eq. (4.3).

|            | HF     | RPA    | RPA+CUSP |
|------------|--------|--------|----------|
| Energy (10^{-2} eV per electron) | 2.95   | 1.94   | -0.59    |
| Std. dev. (10^{-4} eV per electron) | 2.79   | 2.60   | 0.50     |

TABLE II. VQMC local energy averages and standard deviations of the inhomogeneous system considered in Sec. [IVC]. The HF trial function has no Jastrow factor. The RPAI trial function includes a Jastrow factor containing the homogeneous RPA $u$ function from Eq. (4.2) but no $\chi$ function. The RPAII trial function uses the full inhomogeneous RPA Jastrow factor derived in Sec. [III D].

|            | HF     | RPAI   | RPAII   |
|------------|--------|--------|---------|
| Energy (10^{-2} eV per electron) | -12.24 | -5.8   | -13.32  |
| Std. Dev. (10^{-4} eV per electron) | 4.0    | 4.4    | 3.6     |

TABLE III. VQMC local energy averages and standard deviations of the system considered in Sec. [IVC]. Results for three different trial wave functions are shown. The HF trial function has no Jastrow factor. The EW trial function includes the Ewald-summed $u$ function from Eq. (4.3) and an analytic $\chi$ function calculated using Eq. (2.16). The VM trial function uses the same $u$ function but optimizes the Fourier components of $\chi$ using variance minimization.

|            | HF    | EW    | VM   |
|------------|-------|-------|------|
| Energy (10^{-2} eV per electron) | -12.244 | -15.786 | -15.790 |
| Std. Dev. (10^{-5} eV per electron) | 40.0  | 8.2   | 8.4  |
TABLE IV. VQMC local energy averages and standard deviations of the system considered in Sec. IV C. Results for three different trial wave functions are shown. The HF trial function has no Jastrow factor. The RPAI trial function includes the homogeneous RPA $u$ function with Fourier components given by Eq. (4.4) plus a $\chi$ function generated using Eq. (2.16). The RPAII trial function uses the inhomogeneous RPA Jastrow factor from Sec. III D, to which cusps have been added as explained in Sec. III E. The Fourier cutoff $k_n$ was set to 4.95$a_0^{-1}$ in both cases.

|                  | HF    | RPAI  | RPAII |
|------------------|-------|-------|-------|
| Energy ($10^{-2}$eV per electron) | -12.244 | -15.785 | -15.812 |
| Std. Dev. ($10^{-5}$eV per electron) | 40.0   | 12.2   | 11.4   |