Strongly localized quantum crystalline states of the jellium model

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Abstract

We consider a system made up of $N$ electrons interacting with a neutralizing positive background within a cubic box of volume $V$. After dividing the box into $N$ (or $N/2$) cubic cells for the polarized (unpolarized) case, we average the creation field operator over each cell with a suitable weight function and we consider the quantum crystalline states obtained by letting all the average operators act on the vacuum state. These states exclude the possibility that each cell may momentarily contain more than one or two electrons in the polarized or unpolarized case. The expectation value of the Hamiltonian over this class of states is evaluated in the thermodynamic limit and the weight function is chosen in such a way to minimize the expectation value. The involved numerical analysis is explicitly performed with a weight function having a generalized Gaussian shape depending on a parameter. It turns out that the unpolarized and polarized quantum crystalline states yield an energy per particle smaller than the homogeneous Hartree-Fock ones for $r_s > 90$ and $r_s > 28$, respectively. Moreover, for the polarized case, the energy per particle at $r_s = 100$ is -0.01448ryd close to -0.0153530(8)ryd, the best quantum Monte Carlo value [Drummond et al., Phys. Rev.B 69, 085116, (2004)] and this discrepancy measures the correlation contribution neglected in our approximation.

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I. INTRODUCTION

Quantum Coulombian systems determine the properties of common matter but their theoretical investigation is far from being complete. Around the sixties it has been proved that they are H-stable \(^1,^2\) and thermodynamically stable \(^3\) provided that they are overall neutral and all the constituting species with electrical charges of a given sign are made up of Fermions \(^2,^4\). From this result follows that the so-called jellium model \(^5\) of metallic conductors has a fundamental state \(|\Psi_0\rangle\) with eigenvalue \(E_0(N,V)\) such that \(\epsilon_0(n) \equiv E_0(N,V)/N\) exists as function of the particle number density \(n \equiv N/V\) in the thermodynamic limit: \(N \to \infty, V \to \infty\) with \(n\) fixed. Choosing units such that \(\hbar = 1\), the Hamiltonian of the model reads

\[
\hat{H} = \hat{H}_0 + \hat{V} = \sum_k \sum_{s=1}^2 \frac{k^2}{2m} a^\dagger_{k,s} a_{k,s} + \frac{1}{2V} \sum_{k,q,p} \sum_{s,s'=1}^2 \frac{4\pi e^2}{q^2} a^\dagger_{k+q,s} a_{q,s'} a^\dagger_{p-s,s'} a_{p,s} a_{k,s}
\]

where the involved symbols have the standard meaning (see, e.g., section 3 of Ref. \([^6]\)) and the prime on the summation symbol means that the value \(q = 0\) is excluded from the sum, a convention adopted throughout the paper. Wigner \(^5\) evaluated the expectation value of \(\hat{H}\) over the state

\[
|F_u\rangle \equiv \prod_{|k| \leq k_F} \prod_{s=1}^2 a^\dagger_{k,s}|0\rangle,
\]

describing the fundamental state of a degenerate Fermi gas of \(N\) (non-interacting) electrons with Fermi momentum \(k_F \equiv (3\pi^2n)^{1/3}\). The resulting energy expression coincides with that obtained the Hartree-Fock (HF) equations under the homogeneity assumption. It reads

\[
\epsilon_{Jl,u}(r_s) \equiv \langle F_u|\hat{H}|F_u\rangle/(Ne^2/2a_0) = \left[\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3} - \frac{3}{2\pi r_s}\left(\frac{9\pi}{4}\right)^{1/3}\right] = \frac{2.21}{r_s^2} - 0.916/r_s^4
\]

where \(r_s \equiv r_0/a_0, \quad a_0 \equiv 1/me^2, \quad r_0 = (3/4\pi n)^{1/3} = (9\pi/4)^{1/3}/k_F\), \(r_s\) being the perturbative parameter and \(m\) the electron mass. On general grounds one has

\[
\epsilon_o(r_s) = \epsilon_{Jl,u}(r_s) + \epsilon_{corr,u}(r_s),
\]
where $\epsilon_{\text{corr},u}(r_s)$ denotes the sum of the remaining terms in the perturbative expansion. It obeys the inequality $\epsilon_{\text{corr},u}(r_s) < 0$ and is named correlation energy. Its evaluation is by no way easy. In fact, no further progress in its analytical knowledge was made since papers \cite{7-12} that yielded the expression

$$
\epsilon_{\text{corr},u}(r_s) = 0.0622 \ln r_s - 0.094 + 0.018 r_s \ln r_s
- 0.020 r_s + O(r_s^2 \ln r_s),
$$

(6) the last addend being the most recently evaluated one \cite{12}. Expression (6) can only be accurate for dense systems, because at low density it becomes positive and violates the reported inequality. Even though $\epsilon_{\text{cor}}(r_s)$ is practically unknown from an analytical point of view, it is expected to be small in comparison to Eq. (3). In fact, on the one hand the minimum of Eq. (3) and the corresponding $r_s$ value compare favourably with the ionization energy and the $r_s$ value of metallic sodium \cite{6}. The same happens for the bulk moduli and the cohesive energies of some typical metals (see table 2.2 of Ref. \cite{13} and table 5.3 of \cite{14}). On the other hand, density functional theory (DFT) \cite{15} and quantum Monte Carlo (QMC) calculations \cite{16-22} nowadays provide accurate numerical approximations of the correlation energy that definitely results to be small in comparison to Eq. (3) [see Figs. 1 and 2]. This property also applies to the polarized jellium. In fact, Bloch \cite{23} showed that, if the fundamental state of the jellium is assumed to be fully polarized, the simple HF approximation of the energy per particle is

$$
\epsilon_{\text{el},p}(r_s) = \frac{2^{2/3} 2.21}{r_s^2} - \frac{2^{1/3} 0.916}{r_s}.
$$

(7) This energy becomes smaller than Eq. (3)’s as $r_s > 5.7$. Thus one expects that the jellium, as its density decreases, passes from the unpolarized to the polarized state. Moreover, at low densities, both Eq. (3) and Eq. (7) yield an energy per particle greater than that of ionic crystals. This observation led Wigner \cite{5} to suggest that, at low density, the jellium becomes a crystal (known as Wigner crystal) in the sense that each of its electrons oscillates around its equilibrium position, forming in this way a lattice of harmonic oscillators. In fact, under the assumptions that the crystalline structure is a bcc one and that the harmonic oscillators are decoupled, Wigner \cite{24} obtained the following energy per particle

$$
E_{\text{crst}}/(Ne^2/2a_0) = -\frac{1.79}{r_s} + \frac{3}{r_s^{3/2}}, \quad r_s \gg 1.
$$

(8)
FIG. 1: The energy per particle of the jellium model (in Rydberg units) in the inner part of the $r_s$-range according to different approximations. Unpolarized case: Eq. (3) $\rightarrow$ dotted curve, QMC results$^{21} \rightarrow$ full circles; SLQCS $\rightarrow$ long-dashed curve. Polarized case: Eq. (7) $\rightarrow$ dot-short-dash; Eq. (9) $\rightarrow$ dot-long-dash; QMC results$^{21} \rightarrow$ full triangles: SLQCS $\rightarrow$ continuous curve.

Carr$^{25}$ improved this analysis taking into account the coupling among the oscillators and (leaving aside a further small positive $O(r_s^{-2})$ term) found that

$$E_{crst}/(Ne^2/2a_0) = -\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}}, \quad r_s \gg 1.$$  \hspace{1cm} (9)

Both expressions are definitely smaller than Eq.s (3) and (7) at large $r_s$ (see Figs. 1 and 2). For a reason explained below, this finding would not have been sufficient to conclude that Wigner’s suggestion holds true. This conclusion only follows from the fact that DFT$^{26}$ and QMC analyses$^{17,18,20-22}$ definitely showed that, at high dilution (i.e. $r_s > 106 \pm 1$ according to the most recent QMC analysis$^{22}$), the stable phase of the jellium model is the fully polarized bcc one. Hence, Wigner’s idea that the low density jellium model has a crystalline structure presently can be considered fully established. In passing we mention that this idea has recently found further applications in relating two-dimensional Wigner crystals in presence of a strong magnetic field to quantum Hall effects$^{27-29}$. The reason why Wigner’s conclusion cannot be drawn from the fact that the energies predicted by Eqs. (8) and (9) are smaller
than that of Eq. (7) is related to the fact that, in deriving Eqs. (8) or (9), Wigner and Carr respectively substituted Hamiltonian (1) with that of $N$ appropriate uncoupled or coupled oscillators plus an appropriate constant. By so doing, the Hamiltonians do not coincide with Eq. (1) and one no longer can invoke Rayleigh-Ritz’ principle to conclude that the quantum state associated to the crystalline picture is closer than Eq. (7)’s to the true fundamental state. This appears even more evident from the fact that the energies predicted by Eqs. (8) and (9) are smaller than Eq. (7)’s throughout the full $r_s$ range. In principle, to show that at low density the fundamental state of (1) corresponds to that of a crystal, one should show that the minimum expectation value of $\hat{H}$ only occurs over an appropriate normalized quantum crystalline state $|\Psi_{cr,0}\rangle$. Of course, this would correspond to exactly solve the problem. This being - if not impossible - very hard, one has to confine himself to look for a quantum crystalline state such that the expectation value of $\hat{H}$ on it is smaller than that over state $|F_u\rangle$. Actually, this has already been done in Ref.[30] by solving the HF equations for a Wigner crystal due to the fact that the HF equations coincide with equations obtained minimizing the expectation value of $\hat{H}$ over a determinantal wave-function. In this paper we shall provide a different procedure that, based on Rayleigh-Ritz’s principle and quantum
field theory, allows us to determine a quantum crystalline state with an energy smaller than homogeneous HF’s. To this aim, in section IIA, we shall first average the creation field operator \( \hat{\psi}^\dagger_\alpha(r) \) over each cell of the crystal with a weight function \( \nu(r) \) having the crystal periodicity. Denoting the resulting operators by \( \hat{\psi}^\dagger_{\alpha,m} \), these obey the Jordan-Wigner algebra [see Eq.s (13), (16) and (17)]. Hence, the Rayleigh-Ritz principle is applied to the class of normalized antisymmetric quantum crystalline states \( |\Psi_{cr}\rangle \equiv \prod_{m,\alpha} \hat{\psi}^\dagger_{\alpha,m} |0\rangle \) to determine the unknown \( \nu(r) \) that, in turn, determines the electron density function \( n(r) \). These \( |\Psi_{cr}\rangle \)s will be named strongly localized quantum crystalline states (SLQCS) because they neglect the possibility that two or more electrons may momentarily be present in the same cell. Then, the expectation value of the kinetic and potential operators are evaluated over the SLQCS in terms of the electron density in sects. II.B and II.C for the unpolarized case and in sect. III for the polarized one. The requirement that the resulting expectation value of \( \hat{H} \) be minimum determine the equations that determine \( n(r) \). In sect. IV we show that these equations coincide with the HF ones with a different boundary condition and this implies that exchange and correlation contributions are equal to zero so that electron interactions are not fully accounted for. Aiming to avoid, as far as possible, computer calculations we do not attempt to solve the mentioned equations. We simply consider a family of electron density functions, depending on a parameter \( \alpha \), and numerically evaluate the expectation value of \( \hat{H} \) by the formulae derived in sects. II and III over a grid of \( \alpha \) values. Then, for each \( r_s \) value, we look for the \( \alpha \) value which makes the expectation value of \( \hat{H} \) minimum. The results of this analysis are partly shown in Figs. 1 and 2 and discussed in more detail in sect. V through their comparison with HF and QMC values. Our final conclusions are drawn in sect. VI.

II. BASIC RELATIONS

A. Strongly localized quantum crystalline states

In order to construct a quantum state that describes the electrons in a crystalline configuration we shall proceed as follows. At first we shall assume that the electrons are confined within a cubic box (centered at the origin of a Cartesian frame) of edge \( L \) and volume \( V = L^3 \), and that the system is not polarized. The cube is divided into \( M_c^3 \) cubic cells of
edge $a$ where $M_c$ denotes the number of cells along Cartesian axes $x$, $y$ and $z$ (or $x_i$, with $i = 1, 2, 3$). To relate the values of $M_c$ and $a$ to $N$ and $V$ we need some preliminary remarks. Each cell generally contains two electrons, respectively with spin up and down, in order to fulfill the unpolarization condition. This condition can exactly be fulfilled only if $N/2 = M_c^3$. It is however clear that this restriction fades away in the thermodynamic limit. In fact, one can generally write $N = 2M_c^3 + N_r$ where $M_c$ is the largest positive integer such that the previous relation holds true with $N_r \geq 0$ and integer. According to the above relation, $2M_c^3$ electrons are accommodated in the $M_c^3$ cells that together form the outset cubic box $V$, while the remaining $N_r$ electrons will be located in $N_r/2$ or $N_r/2 + 1$ (depending on whether $N_r$ is even or odd) cells next to the external boundary of $V$. Recalling that the electric total charge of each cell (but one, if $N_r$ is odd) is equal to zero, the contribution of these border cells becomes negligible in the thermodynamic limit (see pages 402-404 of Ref. [13]). As $N \to \infty$ we have that $M_c \to \infty$ and from the above considerations follows that the lattice spacing is

$$a = L/M_c \approx L(2/N)^{1/3} = (8\pi/3)^{1/3}r_0.$$ (10)

For notational simplicity, in the following we explicitly refers to the case of odd $M_c$ so as to write $M_c = 2M + 1$. Then, $V_m$, the $m[≡ (m_1, m_2, m_3)]$th cell of $V$, is defined as

$$V_m \equiv \{ r \mid (m_i - \frac{1}{2})a < x_i < (m_i + \frac{1}{2})a, \quad m_i = -M, \ldots, M, \quad i = 1, 2, 3 \}.$$ (11)

By construction,

$$V = \bigcup_{-M \leq m_1, m_2, m_3 \leq M} V_m = \bigcup_{m \in \mathbb{Z}_V^3} V_m$$ (12)

where $\mathbb{Z}_V^3 \equiv \mathbb{Z}^3 \cap V$ is the intersection of the cubic three-dimensional lattice $\mathbb{Z}^3$ of spacing $a$ with the outset box $V$. Introduce now the operators

$$\hat{\psi}_{\alpha, m} \equiv \int_{V_m} \nu(r)\hat{\psi}_{\alpha}(r) dv, \quad \hat{\psi}_{\alpha, m}^\dagger \equiv \int_{V_m} \overline{\nu}(r)\hat{\psi}_{\alpha}^\dagger(r) dv,$$ (13)

obtained averaging the electron field operators of destruction and creation over the $m$th cell respectively with a weight function $\nu(r)$ and its complex conjugate $\overline{\nu}(r)$. Function $\nu(r)$ is assumed to be periodic with period $a$, i.e.

$$\nu(r) = \nu(r + am),$$ (14)
m being an arbitrary triple of relative integers. Moreover we also require that \( \nu(r) \) and all its first partial derivatives are continuous throughout the closed unit cell and, finally, that \( \nu(r) \) has unit norm over the unit cell, i.e.

\[
\int_{V_m} |\nu(r)|^2 dv = 1.
\]  

(15)

Definitions (13) and the canonical anticommutation relation of fields \( \hat{\psi}_\alpha \) and \( \hat{\psi}_\alpha^\dagger \) yield the following anticommutation relations

\[
\{ \hat{\psi}_{\alpha,m}, \hat{\psi}_{\beta,m'}^\dagger \} = \delta_{\alpha,\beta} \delta_{m,m'},
\]

(16)

\[
\{ \hat{\psi}_{\alpha,m}, \hat{\psi}_{\beta,m'} \} = \{ \hat{\psi}_{\alpha,m}^\dagger, \hat{\psi}_{\beta,m'}^\dagger \} = 0.
\]

(17)

One immediately verifies that the state \( \hat{\psi}_{\alpha,m}^\dagger |0\rangle \) contains one electron within the \( m \)th cell with spin up or down depending on whether \( \alpha \) equals one or two. Furthermore, the expectation value of the particle number density operator \( \hat{n}(r) \) over the previous state is

\[
\langle 0 | \hat{\psi}_{\alpha,m} \hat{n}(r) \hat{\psi}_{\alpha,m}^\dagger |0 \rangle = |\nu(r)|^2 \Theta(r \in V_m)
\]

\[
\equiv n(r) \Theta(r \in V_m),
\]

(18)

where, similarly to Heaviside’s function definition, \( \Theta(r \in V_m) \) is defined to be equal to one or zero depending on whether the tip of \( r \) lies within or outside \( V_m \). Eq. (18) shows that \( n(r) \), the square modulus of function \( \nu(r) \) entering definition (13), times \( \Theta(r \in V_m) \) is the particle number density of the electrons within the full box for the quantum state \( \hat{\psi}_{\alpha,m}^\dagger |0\rangle \).

Consider now the fully antisymmetric state

\[
|W_{cr}\rangle \equiv \left( \prod_{-M \leq m_1, m_2, m_3 \leq M} \prod_{\alpha=1}^{2} \hat{\psi}_{\alpha,m}^\dagger \right) |0\rangle
\]

(19)

and label the index pair \((\alpha, m)\) by a single index \( J \) that runs over \( \{1, \ldots, N\} \). Then Eq. (19) is more compactly written as

\[
|W_{cr}\rangle \equiv \left( \prod_{J=1}^{N} \hat{\psi}_{J}^\dagger \right) |0\rangle.
\]

(20)

One easily verifies that \( \langle W_{cr} | \hat{n}(r) | W_{cr} \rangle = n(r) \) [the latter’s value on the cells’ boundaries being defined by continuity]. Hence, quantum state \( |W_{cr}\rangle \) describes an unpolarized crystalline configuration of the \( N \) electrons within the cubic box \( V \) with a periodic density \( n(r) = |\nu(r)|^2 \). It should be noted that the states of form (19) have a peculiar feature: they do
not allow that two (or more) creation field operators, with the same spin, act on the same cell. This limitation will be discussed in more detail at the end of section IV. As already anticipated, quantum states of form (20) are named strongly localized quantum crystalline states (SLQCS). Despite this fact, it looks reasonable that at high dilution the fundamental state of the jellium model is closer to a SLQCS than to Eq. (2). Our task now is to find function $\nu(r)$ and the parameter region where the above property is fulfilled. This will be accomplished by: i) evaluating the expectation value of (1) over $|W_{cr}\rangle$, ii) performing the thermodynamic limit, iii) deriving the equations that determine the $\nu(r)$ function that minimizes the expectation value and iv) approximately solving the last equations so as to make the comparison of the resulting energy with homogeneous HF’s possible.

The evaluation of $\langle W_{cr}|\hat{H}|W_{cr}\rangle$ requires that of $\langle W_{cr}|\hat{T}|W_{cr}\rangle$ and $\langle W_{cr}|\hat{V}|W_{cr}\rangle$, where

$$
\hat{T} = \hat{H}_0 = \int_V \frac{(\nabla \hat{\psi}_\alpha^\dagger(r) \cdot \nabla \hat{\psi}_\alpha(r))}{2m} dv = -\int_V \frac{\hat{\psi}_\alpha^\dagger(r) \cdot \nabla^2 \hat{\psi}_\alpha(r)}{2m} dv \quad (21)
$$

and

$$
\hat{V} \equiv \frac{e^2}{2V} \sum'_{k,p,q} \sum'_{s,s'=1}^2 \frac{4\pi}{q^2} a_{k+q,s}^d a_{p-q,s'}^d a_{p,s'} a_{k,s} \quad (22)
$$

B. Evaluation of the expectation value of $\hat{T}$

The evaluation of $\langle W_{cr}|\hat{T}|W_{cr}\rangle$ is easily performed by the following anticommutation relations

$$
\{\hat{\psi}_\alpha(r), \hat{\psi}_\beta^\dagger(r)\} = \delta_{\alpha,\beta} \Theta(r \in V_m), \quad \alpha, \beta = 1, 2, \quad m \in \mathbb{Z}^3 \quad (23)
$$

and

$$
\{\hat{\psi}_\alpha^\dagger(r), \hat{\psi}_\beta(r)\} = \delta_{\alpha,\beta} \nu(r) \Theta(r \in V_m), \quad \alpha, \beta = 1, 2, \quad m \in \mathbb{Z}^3 \quad (24)
$$

the remaining anticommutators being equal to zero, i.e.

$$
\{\hat{\psi}_\alpha(r), \hat{\psi}_\beta(r)\} = \{\hat{\psi}_\alpha^\dagger(r), \hat{\psi}_\beta^\dagger(r)\} = 0 \quad (25)
$$
By the relabel \((\beta, m) \rightarrow J\) the above anticommutators are more compactly written as

\[
\{\hat{\psi}_\alpha(r), \hat{\psi}^\dagger_J\} = F_{\alpha, J}(r) \equiv \delta_{\alpha, \beta} \mathcal{P}(r) \Theta(r \in V_m), \tag{26}
\]

\[
\{\hat{\psi}^\dagger_J(r), \hat{\psi}_\beta\} = \overline{F}_{\alpha, J}(r),
\]

with \(J = 1, \ldots, N\) and \(\alpha = 1, 2\). The subsequent use of Eqs. (26) and (20) yields

\[
\hat{\psi}_\alpha(r)|W_{cr}\rangle = \sum_{J=1}^{N} (-1)^{J-1} \hat{\psi}^\dagger_1 \cdots \hat{\psi}^\dagger_{J-1} F_{\alpha, J}(r) \times \hat{\psi}^\dagger_{J+1} \cdots \hat{\psi}^\dagger_N |0\rangle. \tag{27}
\]

Its adjoint determines \(|W_{cr}|\hat{\psi}^\dagger_\alpha(r)\rangle\). In this way, by Eqs. (16), one finds that

\[
\langle W_{cr} | \nabla \hat{\psi}^\dagger_\alpha(r) \cdot \nabla \hat{\psi}_\alpha(r) | W_{cr} \rangle = \sum_{J, J' = 1}^{N} (-1)^{J+J'-2} \times \frac{\nabla \overline{F}_{\alpha, J}(r) \cdot \nabla F_{\alpha, J}(r)}{2M} \times \langle 0 | \hat{\psi}_N \cdots \hat{\psi}_{J+1} \hat{\psi}_{J+1} \cdots \hat{\psi}_1 \hat{\psi}^\dagger_{J-1} \hat{\psi}^\dagger_{J+1} \cdots \hat{\psi}^\dagger_N |0\rangle
\]

\[
= \sum_{J = 1}^{N} \frac{\nabla \overline{F}_{\alpha, J}(r) \cdot \nabla F_{\alpha, J}(r)}{2M} \times \langle 0 | \hat{\psi}_N \cdots \hat{\psi}_{J+1} \hat{\psi}_{J+1} \cdots \hat{\psi}_1 \hat{\psi}^\dagger_{J-1} \hat{\psi}^\dagger_{J+1} \cdots \hat{\psi}^\dagger_N |0\rangle
\]

\[
= \sum_{J = 1}^{N} \frac{\nabla \overline{F}_{\alpha, J}(r) \cdot \nabla F_{\alpha, J}(r)}{2M} = \sum_{m \in \mathbb{Z}^3 \cap V} \frac{\nabla \mathcal{P}(r) \cdot \nabla \nu(r)}{2M} \Theta(r \in V_m) \delta_{\alpha, \beta} \delta_{\alpha, \beta}. \tag{28}
\]

In obtaining the last relation, we converted \(J\) to \((\beta, m)\) and used Eq. (26). Finally, in the thermodynamic limit, the periodicity of \(\nu(r)\) yields the sought for expression of the \(\hat{T}\) expectation value

\[
\langle W_{cr} | \hat{T} | W_{cr} \rangle = \frac{N}{2M} \int_{V_0} |\nabla \nu(r)|^2 dv, \tag{29}
\]

where \(V_0\) is the cell defined by Eq. (11) with \(m = 0\). It is now convenient to introduce the following dimensionless quantities

\[
\tilde{\xi} \equiv 2r/a, \quad \text{and} \quad \nu_1(\tilde{\xi}) \equiv (a/2)^{3/2} \nu(a \tilde{\xi}/2) = (a/2)^{3/2} \nu(r). \tag{30}
\]

\(\tilde{\xi}\) is a dimensionless position vector such that the largest and smallest value of each of its components respectively are +1 and -1 as \(r\) ranges over cell \(V_0\). In this way, \(\tilde{\xi}\) is confined to
vary within the cubic cell \( V_0 \) (different from \( V_0 \)) defined as
\[
V_0 \equiv \{ \xi | -1 < \xi, < 1, i = 1, 2, 3 \}.
\] (31)

By Eqs. (30) and (15) it results that \( \nu_1(\xi) \) has unit norm over \( V_0 \). Further, \( \nu_1(\xi) \) can be defined throughout \( R^3 \) imposing the periodicity condition \( \nu_1(\xi) = \nu_1(\xi + 2m) \). In terms of the just defined dimensionless quantities Eq. (29) becomes
\[
\langle W_{cr} | \hat{T} | W_{cr} \rangle = Ne^2 \frac{1}{2a_0 r_s^2} \left( \frac{3}{\pi} \right)^{2/3} \int_{V_0} |\nabla \xi \nu_1(\xi)|^2 d^3 \xi
\] (32)
by Eqs. (32) and (10).

**C. Evaluation of the expectation value of \( \hat{V} \)**

We find it advantageous to start from expression (22) of \( \hat{V} \) because this accounts for the contribution of the positive background through the fact that the mode \( q = 0 \) is excluded in the first sum of Eq. (22). Using the decomposition
\[
\hat{\psi}_\alpha(r) = \sum_k \sum_{s=1}^2 \frac{e^{ik \cdot r}}{\sqrt{\Omega}} a_{k,s} \eta_{\alpha}^s,
\] (33)
from Eq. (13) one obtains
\[
\hat{\psi}_{\alpha,m} = \sum_k \sum_{s=1}^2 \frac{a_{k,s} \eta_{\alpha}^s}{\sqrt{\Omega}} \int_{V_m} e^{ik \cdot r} \nu(r) dv.
\] (34)
The Fourier transform (FT) of \( \nu(r) \), restricted to the unit cell centered at the origin, is defined as
\[
\tilde{\nu}(k) \equiv \int_{V_0} \nu(r) e^{-ik \cdot r} dv,
\] (35)
and obeys
\[
\overline{\tilde{\nu}(k)} = \tilde{\nu}(-k)
\] (36)
where, hereafter, the tilde denotes the FT and the overbar the complex conjugate. The periodicity of \( \nu(r) \) allows us to write the integral present in Eq. (34) as \( e^{iak \cdot m} \tilde{\nu}(-k) \), so that \( \hat{\psi}_{\alpha,m} \) reads
\[
\hat{\psi}_{\alpha,m} = \hat{\psi} J = \sum_{k,s} \varphi J_{k,s} a_{k,s},
\] (37)
where we have put
\[ \varphi_{J,k} = e^{i\int_k^0 pL^2} \sqrt{V}. \] (38)

From Eq. (37), its adjoint and the canonical anticommutation relations one finds that
\[ \{a_{k,s}, \hat{\psi}_J\} = \varphi_{J,k,s} \quad \text{and} \quad \{a_{k,s}, \hat{\psi}^+_J\} = \overline{\varphi}_{J,k,s}. \] (39)

By these relations the evaluation of \( \langle W_{cr} | \hat{V} | W_{cr} \rangle \) becomes straightforward. In fact,
\[ a_{k,s} | W_{cr} \rangle = \sum_{J=1}^{N} (-1)^{J-1} \hat{\psi}^+_1 \ldots \hat{\psi}^+_J \overline{\varphi}_{J,k,s} \times \hat{\psi}^+_J \ldots \hat{\psi}^+_N | 0 \rangle \] (40)
and
\[ a_{p,s'} a_{k,s} | W_{cr} \rangle = \sum_{J=1}^{N} \sum_{L=1}^{J-1} (-1)^{J+L-2} \overline{\varphi}_{L+p,s'} \overline{\varphi}_{J,k,s} \times \hat{\psi}^+_1 \ldots \hat{\psi}^+_L \hat{\psi}^+_1 \ldots \hat{\psi}^+_L \overline{\varphi}_{J+1,k,s} \times \hat{\psi}^+_J \ldots \hat{\psi}^+_N | 0 \rangle, \] (41)
where it is understood that appended index values can neither be smaller than one nor exceed \( N \). The above expression can be recast in the form
\[ a_{p,s'} a_{k,s} | W_{cr} \rangle = \sum_{J=1}^{N} \sum_{L=1}^{J-1} (-1)^{J+L} \overline{\varphi}_{L+p,s'} \overline{\varphi}_{J,k,s} \times \hat{\psi}^+_1 \ldots \hat{\psi}^+_L \hat{\psi}^+_1 \ldots \hat{\psi}^+_L \overline{\varphi}_{J+1,k,s} \times \hat{\psi}^+_J \ldots \hat{\psi}^+_N | 0 \rangle \] (42)
and the prime over the product means that index \( \mathcal{M} \) never takes values \( J \) and \( L \). By relation (42) and its adjoint one gets
\[ \langle W_{cr} | a_{k+q,s}^+ a_{p-q,s'} a_{p,s'} a_{k,s} | W_{cr} \rangle = \sum_{J', J=1}^{N} \sum_{L'=1}^{J'-1} \sum_{L=1}^{J+L} \times (-1)^{J'+L'+J+L} \varphi_{J';k+q,s'} \varphi_{L;p-q,s'} \overline{\varphi}_{J,k,s} \overline{\varphi}_{J,p,s'} \overline{\varphi}_{L,k,s} \overline{\varphi}_{J+p,s'} \times \langle W_{cr} | \hat{\psi}^+_J \hat{\psi}^+_1 \hat{\psi}^+_L \hat{\psi}^+_1 \hat{\psi}^+_L \hat{\psi}^+_J \hat{\psi}^+_1 \hat{\psi}^+_L \hat{\psi}^+_J \hat{\psi}^+_1 \hat{\psi}^+_L \ldots \hat{\psi}^+_N | W_{cr} \rangle. \] (43)
The matrix elements are different from zero only if $J' = J$ and $L' = L$ and, in this case, they are equal to one. Thus, one finds that

$$
\langle W_{cr}|a_{k+q,s}^\dagger p_{-q,s'}^\dagger a_{p,s'} a_{k,s}|W_{cr}\rangle
= \sum_{J=1}^{N} \sum_{L=1}^{J-1} (\varphi_{J,k,s} \varphi_{L,p,s} - \varphi_{L,k,s} \varphi_{J,p,s'}) \times
\left( \varphi_{J,k+q,s'} \varphi_{L,p-2q,s} - \varphi_{L,k+q,s'} \varphi_{J,p-2q,s} \right).
$$

The terms in the above sums are symmetric with respect to the exchange $J \leftrightarrow L$ and equal to zero if $J = L$. Thus, we can let $L$ range over $1, \ldots, N$ provided that we divide the result by two. Converting $J$ and $L$ to index pairs $(\alpha, m)$ and $(\alpha', m')$, using definition (38) and performing the sums over $\alpha$ and $\alpha'$ one finds that

$$
\langle W_{cr}|a_{k+q,s}^\dagger p_{-q,s'}^\dagger a_{p,s'} a_{k,s}|W_{cr}\rangle
= \tilde{\nu}(\tilde{k} - q) \tilde{\nu}(\tilde{q} - p) \tilde{\nu}(\tilde{k}) \tilde{\nu}(\tilde{p}) \times
\sum_{m, m' \in \mathbb{Z}^3} \left[ \delta_{s, s'} \delta_{s, s'} \left( e^{iaq \cdot (m - m')} + c.c. \right)
- \delta_{s, s} \delta_{s, s'} \left( e^{ia(k - p + q) \cdot (m - m')} + c.c. \right) \right],
$$

where $c.c.$ stands for complex conjugate. Each sum present in the above expression is the product of three sums of the form

$$
\sum_{m=-M}^{M} \sum_{m'=-M}^{M} e^{iaq \cdot (m - m')}.
$$

One easily verifies that

$$
\sum_{m=-M}^{M} \sum_{m'=-M}^{M} e^{iap \cdot (m - m')} = (2M + 1) \times
\sum_{p=-2M}^{2M} e^{iap} - \sum_{p=-2M}^{2M} \frac{|p|}{2M + 1} e^{iap}.
$$

In the limit $M \to \infty$ one finds that

$$
\sum_{m=-M}^{M} \sum_{m'=-M}^{M} e^{iaq \cdot (m - m')} \approx (2M + 1) \sum_{p=-\infty}^{\infty} e^{iap}
= (2M + 1) 2\pi \sum_{m=-\infty}^{\infty} \delta(aq - 2m\pi).
$$
In the three dimensional case, recalling that \((N/2)^{1/3} = M_c = (2M + 1)\), one has
\[
\sum_{m,m' \in \mathbb{Z}^3} e^{i\mathbf{a q} \cdot (\mathbf{m} - \mathbf{m}') \approx \frac{N(2\pi)^3}{2} \sum_{\mathbf{m} \in \mathbb{Z}^3} \delta(\mathbf{a q} - 2\pi \mathbf{m}). \quad (49)
\]
Consequently, Eq. (45) becomes
\[
\langle \mathbf{W}_{cr} | a^\dagger_{k+\mathbf{q},s} a^\dagger_{p-\mathbf{q},s'} a_{p,s'} a_{k,s} | \mathbf{W}_{cr} \rangle \\
\approx (2\pi)^3 N \hat{\nu}(-\mathbf{k} - \mathbf{q}) \hat{\nu}(\mathbf{q} - \mathbf{p}) \hat{\nu}(-\mathbf{k}) \hat{\nu}(-\mathbf{p}) \times \\
\sum_{\mathbf{m} \in \mathbb{Z}^3} \left[ \delta_{s,s} \delta_{s,s'} \delta(\mathbf{a q} - 2\pi \mathbf{m}) \\
- \delta_{s,s'} \delta_{s,s} \delta(\mathbf{a (k + q - p) - 2\pi m}) \right]. \quad (50)
\]
By this result, in the limit \(V \to \infty\) the expectation value of \(\hat{V}\) becomes
\[
\langle \mathbf{W}_{cr} | \hat{V} | \mathbf{W}_{cr} \rangle = \frac{e^2 N}{4(2\pi)^6} \times \\
\int d^3p \, d^3k \, d^3q \frac{4\pi \hat{\nu}(\mathbf{k} + \mathbf{q}) \hat{\nu}(\mathbf{p} - \mathbf{q}) \hat{\nu}(\mathbf{k}) \hat{\nu}(\mathbf{p})}{q^2} \times \\
\left[ 4 \sum_{\mathbf{m} \in \mathbb{Z}^3} \delta(\mathbf{a q} - 2\pi \mathbf{m}) - 2 \sum_{\mathbf{m} \in \mathbb{Z}^3} \delta(\mathbf{a (k + q - p) - 2\pi m}) \right] \tag{51}
\]
where the value \(\mathbf{m} = \mathbf{0}\) is excluded in the first sum because value \(\mathbf{q} = \mathbf{0}\) is not allowed in Eq. (22), and the numerical factors in front of the sums account for the sum over \(s\) and \(s'\).

After introducing the dimensionless momenta
\[
\mathbf{P} \equiv \frac{\mathbf{a p}}{2}, \quad \mathbf{K} \equiv \frac{\mathbf{a k}}{2}, \quad \text{and} \quad \mathbf{Q} \equiv \frac{\mathbf{a q}}{2}, \quad (52)
\]
from Eqs. (35) and (30) one obtains that
\[
\hat{\nu}_1(\mathbf{K}) = \int_{\tilde{\mathbf{q}}} e^{-i\tilde{\mathbf{K}} \tilde{\mathbf{q}}} \nu_1(\tilde{\mathbf{q}}) d^3\tilde{\mathbf{q}} = \left( \frac{2}{a} \right)^{3/2} \hat{\nu}(\mathbf{k}). \quad (53)
\]
After putting
\[
n_1(\tilde{\mathbf{q}}) = |\nu_1(\tilde{\mathbf{q}})|^2 = (a/2)^3 n(\mathbf{r}), \tag{54}
\]
where the last equality follows from Eq. (30) and the fact that \(n(\mathbf{r}) = |\nu(\mathbf{r})|^2\), one easily shows that the following relations
\[
\int \hat{\nu}_1(\mathbf{K} + \mathbf{P}) \hat{\nu}_1(\mathbf{K}) d^3K = (2\pi)^3 \int_{\tilde{\mathbf{q}}} e^{i\mathbf{P} \cdot \tilde{\mathbf{q}}} |\nu_1(\tilde{\mathbf{q}})|^2 d^3\tilde{\mathbf{q}} = (2\pi)^3 \tilde{n}_1(-\mathbf{P}) \tag{55}
\]
and

\[
\sum_{m \in \mathbb{Z}^3} \bar{\nu}(P + \pi m) \nu(P - Q + \pi m)
\]

\[
= 8 \int_{V_0} |\nu_1(\xi)|^2 e^{-iQ \cdot \xi} d^3 \xi = 8 \tilde{n}_1(Q)
\]

hold true. By Eqs. (52), (55), (56) and (10), Eq. (51) converts into

\[
\langle W_{cr} | \hat{V} | W_{cr} \rangle = \frac{Ne^2}{2a_0 r_s \pi} \left( \frac{3}{\pi} \right)^{1/3} \times
\]

\[
\left[ \sum_{m \in \mathbb{Z}^3} \frac{\tilde{g}_1(\pi m)^2}{|m|^2} - \frac{1}{2\pi} \int \frac{|\tilde{n}_1(Q)|^2}{|Q|^2} d^3 Q \right].
\]

Define the auto-correlation function of \(n_1(\xi)\) as

\[
g_1(\xi) \equiv \int_{V_0} n_1(\xi + \eta)n_1(\eta) d^3 \eta.
\]

This differs from zero only within the cubic cell centered at the origin and with edge length equal to four. This cell will be denoted by \(2V_0\). One finds that

\[
\tilde{g}_1(q) \equiv \int_{2V_0} e^{-i\xi \cdot Q} g_1(\xi) d^3 \xi = |\tilde{n}_1(Q)|^2.
\]

Then, recalling that \(4\pi/|Q|^2\) is the FT of \(1/r\), the integral in Eq. (57) can be written as

\[
\int \frac{|\tilde{n}_1(Q)|^2}{|Q|^2} d^3 Q = 2\pi^2 \int_{2V_0} \frac{g_1(\xi)}{|\xi|} d^3 \xi.
\]

Finally, Eq. (57) reads

\[
\langle W_{cr} | \hat{V} | W_{cr} \rangle = \frac{Ne^2}{2a_0 r_s \pi} \left( \frac{3}{\pi} \right)^{1/3} \times
\]

\[
\left[ \sum_{m \in \mathbb{Z}^3} \frac{\tilde{g}_1(\pi m)}{|m|^2} - \pi \int_{2V_0} \frac{g_1(\xi)}{|\xi|} d^3 \xi \right].
\]

### III. FINAL EXPRESSIONS FOR THE UNPOLARIZED AND POLARIZED CASE

In this section we report the final expressions of the expectation value of the Hamiltonian over the quantum crystalline states of the form (20) for the unpolarized and polarized cases. The first case has been analyzed in the previous section. There we found that, if we put

\[
t[\nu_1] \equiv \int_{V_0} |\nabla_\xi \nu_1(\xi)|^2 d^3 \xi,
\]

15
\[ v_d[\nu_1] \equiv \sum_{m \in \mathbb{Z}^3} \frac{\tilde{g}_1(\pi m)}{|m|^2} \]  

(63)

and

\[ v_e[\nu_1] \equiv - \int_{2\pi}\frac{g_1(\xi)}{|\xi|}d^3\xi, \]  

(64)

the expectation value of \( \hat{H} \) over the unpolarized crystalline state defined by Eq. (20) is

\[ c_u[\nu_1, r_s] \equiv \langle W_{cr}|\hat{H}|W_{cr}\rangle_u \left/ \left( N \frac{e^2}{2a_0} \right) \right. \]  

(65)

\[ = \frac{c_t v_d[\nu_1]}{r_s^2} + \frac{c_d v_d[\nu_1]}{r_s} + \frac{c_e v_e[\nu_1]}{r_s} \]

with

\[ c_{t,u} \equiv \left( \frac{3}{\pi} \right)^\frac{2}{3}, \quad c_{d,u} \equiv \frac{1}{\pi} \left( \frac{3}{\pi} \right)^\frac{1}{3}, \quad c_{e,u} \equiv \left( \frac{3}{\pi} \right)^\frac{1}{3}. \]  

(66)

In fact, the first contribution on the right hand side (rhs) of Eq. (65) represents the expectation value of \( \hat{T} \) [see Eq. (32)], while the sum of the remaining two terms is that of \( \hat{V} \) [see Eq. (61)]. It is stressed that expressions (62), (63) and (64) do not explicitly depend on the density of the system because they only involve dimensionless quantities \( \tilde{\xi}, \nu_1(\tilde{\xi}) \) and \( g_1(\tilde{\xi}) \). An implicit dependence is however present in \( \nu_1(\tilde{\xi}) \) and, consequently, in \( n_1(\tilde{\xi}), g_1(\tilde{\xi}) \) and \( \tilde{g}_1(K) \) so as to make the \( r_s \) dependence of \( \langle \Psi_{cr}|\hat{H}|\Psi_{cr}\rangle \) different from that of Eq. (3).

If we assume that the system is fully polarized, each cell exactly contains one electron with, say, spin up. Thus, the number of the cells is determined by the condition \( N = M_c^3 + N_r \) and the lattice constant is

\[ a_p = \frac{L}{M_c} \approx L/N^{1/3} = (4\pi/3)^{1/3}r_0 = a_u/2^{1/3} \]  

(67)

where \( a_u \) denotes now the unpolarized spacing, denoted by \( a \) in Eq. (10). The fully polarized and completely antisymmetric SLQCS becomes

\[ |W_{cr,p}\rangle = \left( \prod_{m \in \mathbb{Z}^3_V} \psi_{1,m}^\dagger \right)|0\rangle \]  

(68)

with \( \mathbb{Z}^3_V \) denoting now the intersection of \( V \) with the cubic lattice of spacing \( a_p \). The calculation of \( \langle W_{cr,p}|\hat{T}|W_{cr,p}\rangle \) and \( \langle W_{cr,p}|\hat{V}|W_{cr,p}\rangle \) proceeds similarly to what we did in sects. II.B and II.C with the difference that relabel \((\alpha, m) \rightarrow J\) becomes now \((1, m) \rightarrow J\). In Eq. (28), this implies that the sum over \( \beta \) no longer is present since we always have \( \beta = 1 \) and that the sum over \( m \) yields \( N \) instead of \( N/2 \). Hence, the numerical factor on the rhs of
Eq. (29) is unchanged. However, when this integral is converted to the relevant dimensionless quantities, the factor $a_u^{-2}$ converts into $a_p^{-2}$. Thus, recalling Eq. (67), numerical factor $c_{t,u}$ in the rhs of Eq. (66) must be multiplied by $2^{2/3}$. In evaluating $\langle W_{cr}|\hat{V}|W_{cr}\rangle_p$, after arriving at expression (44), we must not perform the sums over $\alpha$ and $\alpha'$, both indices being equal to one if spins are assumed to point up. Hence, we are left with quantities $\eta_{s,1}^s = \delta_{s,1}$ and $\eta_{s',1}^s = \delta_{s',1}$ and the sums over $s$ and $s'$ simply yield 1. Consequently, in Eq. (51), we must omit factors 4 and 2 in front of the two sums. Moreover, the cell number instead of $N/2$ becomes $N$ and the lattice parameter $a_u$, present in Eqs. (52) and (53), becomes $a_p$. For these reasons, numerical factors $c_{d,u}$ and $c_{e,u}$ must be multiplied by $2 \cdot 2^{1/3}/4$ and $2 \cdot 2^{1/3}/2$, respectively. In conclusion, the energy per particle in the polarized case is

$$
\epsilon_p[\nu_1, r_s] \equiv \langle W_{cr,p}|\hat{H}|W_{cr,p}\rangle / \left( N \frac{e^2}{2a_0} \right) = \frac{c_{t,p} t[\nu_1]}{r_s^2} + \frac{c_{d,p} v_d[\nu_1]}{r_s} + \frac{c_{e,p} v_e[\nu_1]}{r_s},
$$

with

$$
c_{t,p} \equiv \left( \frac{6}{\pi} \right)^\frac{2}{3}, \quad c_{d,p} \equiv \frac{1}{\pi} \left( \frac{3}{4\pi} \right)^\frac{1}{2}, \quad c_{e,p} \equiv \left( \frac{6}{\pi} \right)^\frac{1}{3}.
$$

### IV. FUNCTIONAL EQUATION FOR $\nu_1(\vec{\xi})$

From Eqs. (65) and (69) it appears evident that the general form of the energy per particle is

$$
\epsilon[\nu_1, r_s] = \frac{c_{t} t[\nu_1]}{r_s^2} + \frac{c_{d} v_d[\nu_1]}{r_s} + \frac{c_{e} v_e[\nu_1]}{r_s},
$$

where we must append to coefficients $c_t$, $c_d$ and $c_e$ further index $u$ or $p$ depending on the polarization of the system. In principle the function $\nu_1$ is determined by the condition that $\epsilon[\nu_1]$ be minimum. For completeness, we derive the equations that follow from this condition. First we observe that $\nu(\vec{\xi})$ can be written as

$$
\nu_1(\vec{\xi}) = \sqrt{n_1(\vec{\xi})} e^{i\omega(\vec{\xi})},
$$

where $\omega(\vec{\xi})$ is a real function. Then, $t[\nu_1]$ can be written as

$$
t[n_1, \omega] = \int_{V_0} [n_1(\vec{\xi}) (\nabla \omega) \cdot (\nabla \omega) + (\nabla \sqrt{n_1}) \cdot (\nabla \sqrt{n_1})] d^3 \xi,
$$

with
while \( v_d[\nu_1] = v_d[n_1] \) and \( v_e[\nu_1] = v_e[n_1] \) since these do not depend on \( \omega(\vec{\xi}) \). Functions \( \omega(\vec{\xi}) \) and \( n_1(\vec{\xi}) \), with \( n_1(\vec{\xi}) \) normalized, are obtained minimizing the functional

\[
\mathcal{E}[n_1, \omega, \lambda] \equiv A t[\nu_1] + B v_d[\nu_1] + C v_e[\nu_1] - \lambda \left( \int_{V_0} n_1(\vec{\xi}) d^3\xi - 1 \right),
\]

where we have put \( A \equiv c_t/r_s^2 \), \( B \equiv c_d/r_s \) and \( C \equiv c_e/r_s \). Thus, \( n_1(\vec{\xi}), \omega(\vec{\xi}) \) and \( \lambda \) are the solutions of the following equations

\[
\frac{\delta \mathcal{E}}{\delta \omega(\vec{\xi})} = 0, \quad \frac{\delta \mathcal{E}}{\delta n_1(\vec{\xi})} = 0, \quad \frac{\partial \mathcal{E}}{\partial \lambda} = \int_{V_0} n_1(\vec{\xi}) d^3\xi - 1 = 0.
\]

Observing that

\[
\frac{\delta t[n_1, \omega]}{\delta \omega(\vec{\xi})} = -2 \left[ n_1(\vec{\xi}) \nabla^2 \omega(\vec{\xi}) + (\nabla n_1) \cdot (\nabla \omega) \right],
\]

\[
\frac{\delta t[n_1, \omega]}{\delta n_1(\vec{\xi})} = (\nabla \omega) \cdot (\nabla \omega) - n_1^{-1/2} \nabla^2 n_1^{1/2},
\]

\[
\frac{\delta g_1(\vec{\xi}')}{\delta n_1(\vec{\xi})} = n_1(\vec{\xi} + \vec{\xi}') + n_1(\vec{\xi} - \vec{\xi}),
\]

the first two equations of (75) respectively convert into

\[
n_1(\vec{\xi}) \nabla^2 \omega(\vec{\xi}) + (\nabla n_1(\vec{\xi})) \cdot (\nabla \omega(\vec{\xi})) = 0,
\]

and

\[
- A \nabla^2 n_1^{1/2}(\vec{\xi}) + An_1^{1/2}(\vec{\xi}) \nabla \omega(\vec{\xi}) \cdot \nabla \omega(\vec{\xi}) + 2B n_1^{1/2}(\vec{\xi}) \sum_{m \in \mathbb{Z}^3} \tilde{n}_1(\pi \vec{m}) \cos(\pi \vec{m} \cdot \vec{\xi}) \frac{1}{|\vec{m}|^2} - C n_1^{1/2}(\vec{\xi}) \int_{2V_0} n_1(\vec{\xi} + \vec{\xi}') + n_1(\vec{\xi} - \vec{\xi}') d^3\xi' = \lambda n_1^{1/2}(\vec{\xi}).
\]

Thus, the SLQCS of form (19) or (68), which yields the minimum expectation value of \( \hat{H} \), is determined by the real functions \( \omega(\vec{\xi}) \) and \( n_1(\vec{\xi}) \) that solve Eqs. (79) and (80) within the cell \( V_0 \) under the further conditions that \( \omega(\vec{\xi}) \) and \( n_1(\vec{\xi}) \) are periodic and that \( n_1(\vec{\xi}) \) is
non-negative and normalized. The periodicity condition can explicitly be accounted for by expanding \( \omega(\vec{\xi}) \) and \( n_1(\vec{\xi}) \) in terms of the complete orthonormal set of functions \( \Phi_m(\vec{\xi}) \equiv e^{im\vec{\xi}/\sqrt{8}} \) and substituting the expansions in the above two equations. We do not report the resulting equations for the coefficients of the expansions because the resulting equations look more involved than Eqs. (79) and (80).

The derivation of Eqs. (79) and (80) coincides with that of the HF equations reported in §2 of [16] because in both cases one minimizes the expectation value of \( \hat{H} \) over a determinantal wave function. However, in contrast with [16], the SLQCS approach assumes that the \( N \) eigenfunctions are now the functions defined as being equal to \( \nu(\vec{\xi} + m) \) inside the \( m \)th cell and zero elsewhere. This fact automatically ensures their orthogonality and explains why Eqs. (79) and (80) involve a single function \( [\nu_1(\vec{\xi})] \) and a single eigenvalue \( [\lambda] \). These considerations deserve a further remark. One would expect that \( \langle W_{cr} | \hat{V} | W_{cr} \rangle \) contains a direct and an exchange term because \( |W_{cr}\rangle \) is a completely antisymmetric state, but the fact that two different eigenfunctions have supports with a void intersection implies that SLQCSs by construction yield exchange and correlation contributions equal to zero.

To better understand the assumptions underlying the SLQCS choice, we observe that a normalized quantum state relevant to \( N \) particles confined to box \( V \) can generally be written as

\[
|\Psi\rangle \equiv \int_{V \otimes N} \frac{\bar{\phi}(\vec{x}_1, \ldots, \vec{x}_N)}{\sqrt{N!}} \hat{\psi}_1^\dagger(\vec{x}_1) \cdots \hat{\psi}_N^\dagger(\vec{x}_N) d\vec{x}_1 \cdots d\vec{x}_N |0\rangle, \tag{81}
\]

where \( \phi(\vec{x}_1, \ldots, \vec{x}_N) \) is a normalized and completely antisymmetric function. (For notational simplicity, we shall confine ourselves to the full polarized case till the end of this section.) The fundamental state is determined by the function \( \phi_0(\vec{x}_1, \ldots, \vec{x}_N) \), implicitly dependent on \( r_s \), that makes the expectation of \( \hat{H} \) over the resulting \( |\Psi_0\rangle \) minimum. In its fundamental state, the system, characterized by a translation invariant Hamiltonian, will have a crystalline behaviour at a given \( r_s \) value if \( \phi_0(\vec{x}_1, \ldots, \vec{x}_N) \) is such that

\[
n(\vec{r}) \equiv \langle \Psi_0 | \hat{n}(\vec{r}) | \Psi_0 \rangle =
N \int_{V \otimes (N-1)} |\phi_0(\vec{r}, \vec{x}_2, \ldots, \vec{x}_N)|^2 d\vec{x}_2 \cdots d\vec{x}_N
\]

turns out to be a periodic function. In this case, state (81) with \( \phi = \phi_0 \) is the exact quantum crystalline fundamental state and the resulting energy will have a null correlation.
contribution. It is straightforward to check that states of form (68) correspond to the choice

\[
\phi_0(x_1, x_2, \ldots, x_N) = \sum_P (-1)^P \times \left( \nu(x_{i_1}) \theta(x_{i_1} \in V_1) \cdots (\nu(x_{i_N}) \theta(x_{i_N} \in V_N) \right),
\]

where the sum runs over all possible permutation of \(\{1, \ldots, N\}\) and \((-)^P\) is the parity of permutation \(\{i_1, \ldots, i_N\}\). According to this relation, function \(\phi_0\) is equal to zero if two or more of its variables fall within the same cell. Consequently, by choosing a SLQCS of form (68) one implicitly assumes that the pair correlation function \(\langle \Psi_{cr,p} | \hat{n}(r_1) \hat{n}(r_2) | \Psi_{cr,p} \rangle\), \(i.e.\) the probability density of finding two particles at two different points \(r_1\) and \(r_2\) is respectively equal to zero or \(n(r_1)n(r_2)\) depending on whether \(r_1\) and \(r_2\) lie in the same or in different cells. This behaviour is radically different from that obtained by (81) that neither factorizes nor, more importantly, vanishes if \(r_1\) and \(r_2\) lie in the same cell. For this reason, the SLQCS approach fails in describing the “fluctuations” in the electron density. One expects that when these are important the SLQCS results will not be accurate. However, in the limit of a very narrow \(n(r)\), the SLQCS aforesaid behaviour is similar to that of an ideal classical crystal with a point-like particle within its unit cell so that the SLQCS description can be realistic only within the \(r_s\) region where the system is crystalline and \(n(r)\) turns out to be rather narrow.

V. A NUMERICAL APPLICATION

Instead of numerically solving Eqs. (79) and (80), which appears to be a rather involved problem, we shall determine the \(r_s\) region where inequality

\[
\langle \Psi_{cr} | \hat{H} | \Psi_{cr} \rangle < \langle F_u | \hat{H} | F_u \rangle
\]

is obeyed confining ourselves to SLQCS defined by a particular class of \(\nu_1(\vec{\xi})\) functions. Clearly, the resulting region will be smaller and the expectation value larger than those obtained by solving Eqs. (79) and (80). Nonetheless, the results appear to be interesting. Hence, we shall assume that \(\nu_1(\vec{\xi})\) has the functional form

\[
\nu_1(\vec{\xi}, \alpha) \equiv G(\xi_1, \alpha)G(\xi_2, \alpha)G(\xi_3, \alpha)
\]
with

\[ G(\xi, \alpha) \equiv C(\alpha)e^{-\alpha \xi^2/(1-\xi^2)}, \quad (86) \]
\[ C(\alpha) \equiv \left( \sqrt{\pi} \Psi\left(\frac{1}{2}, 0; 2\alpha\right) \right)^{-1/2}, \quad (87) \]

where \( \alpha \) is a real positive parameter to be determined by a minimization procedure and \( \Psi\left(\frac{1}{2}, 0; 2\alpha\right) \) is a specialization of \( \Psi(a, c; z) \), the confluent Hypergeometric function defined in §2.5 of Ref. [32]. The reported \( C(\alpha) \) expression ensures that

\[ \int_{-1}^{1} G^2(\xi, \alpha) d\xi = 1. \quad (88) \]

Functional choice (85) implicitly assumes that \( \omega(\vec{\xi}) \equiv 0 \). Further, we assume that \( \nu_1(\vec{\xi}, \alpha) \) is an even non-negative function, fully symmetric in variables \( \xi_1, \xi_2, \xi_3 \), the components of \( \vec{\xi} \) varying within the interval \([-1, 1]\). These assumptions imply that we are considering a crystal with a simple cubic structure. Moreover, functional choice (86) implies that \( \nu_1(\vec{\xi}, \alpha) \) and all its partial derivatives approach zero as \( \vec{\xi} \) approaches the cell boundary. Then, their FTs decrease rather quickly as the momentum increases and the series involving the FTs can safely be truncated. The factorized dependence of \( \nu_1 \) on \( \xi_1, \xi_2 \) and \( \xi_3 \) simplifies some of our results. In particular it results that

\[ t(\alpha) = 6 \int_0^1 \left[dG(\xi, \alpha)\right]^2 d\xi, \quad (89) \]
\[ g_1(\vec{\xi}, \alpha) = \prod_{j=1}^{3} G_1(\xi_j, \alpha), \quad (90) \]
\[ \tilde{g}_1(\pi m, \alpha) = \prod_{j=1}^{3} \left[\tilde{G}^2(\pi m_j, \alpha)\right]^2, \quad (91) \]
\[ v_d(\alpha) = \sum_{m \in \mathbb{Z}^3} \prod_{j=1}^{3} \left[\tilde{G}^2(\pi m_j, \alpha)\right]^2 \frac{1}{|m|^2} \quad (92) \]
\[ v_e(\alpha) = -48 \int_0^2 G_1(\xi_1, \alpha) d\xi_1 \int_0^{\xi_1} G_1(\xi_2, \alpha) d\xi_2 \times \]
\[ \int_0^{\xi_2} \frac{G_1(\xi_3, \alpha)}{\sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}} d\xi_3 \quad (93) \]

where

\[ G_1(\xi, \alpha) = \int_{-1}^{1} G^2(\xi + \xi', \alpha) G^2(\xi', \alpha) d\xi' \quad (94) \]
\[ \tilde{G}^2(q, \alpha) = 2 \int_0^{1} \cos(q \xi) G^2(\xi, \alpha) d\xi. \quad (95) \]
FIG. 3: Left: unpolarized case. Continuous curve: Log$_{10}[c_{u,t}(\alpha)]$ vs. Log$_{10}(\alpha)$; short dash: $c_{d,u}v_d(\alpha)$; dot-dash: $c_{e,u}v_e(\alpha)$; long dash: $c_{d,u}v_d(\alpha) + c_{e,u}v_e(\alpha)$. Right: the same quantities for the polarized case; the horizontal axis values must be shifted by -3. Finally, the two dotted curves show the best $\alpha$ value [as Log$_{10}(\alpha)$ on the horizontal axis, in terms of Log$_{10}(r_s)$, on the vertical axis] for the unpolarized (left) and polarized (right) case, respectively.

The above equations makes it evident that the determination of $t(\alpha)$, $v_e(\alpha)$ and $v_d(\alpha)$ is numerically straightforward. In fact, the integrals must be performed over compact sets where the integrands are continuous while series (91) can safely be truncated because $\tilde{G}^2(q,\alpha)$, as shown in Appendix A, asymptotically decreases as

$$
\tilde{G}^2(q,\alpha) \approx \frac{2\alpha^{1/4}e^{3\alpha/2-\sqrt{2q\alpha}}}{\Psi(1/2,0,2\alpha)q^{3/4}} \sin(q - \sqrt{2q\alpha} + \pi/8).
$$

(96)

In practice, integrals (89), (94) and (95) have been numerically determined considering $10^8$ intermediate points; the $\xi_1,..,\xi_3$ spacing in Eq. (93) was taken equal to $10^{-4}$ and the largest absolute value of each component of $\mathbf{m}$ in Eq. (92) equal to 30. Moreover, quantities $t(\alpha)$, $v_d(\alpha)$ and $v_e(\alpha)$ were evaluated over a grid of $\alpha$ values that span the intervals $(0, 1]$ and $[1, 10]$ with spacings respectively equal to 0.025 and 0.25. The correspondent values are denoted by $t_{a,j} = t_a(\alpha_j)$, $v_{d,a,j}$ and $v_{e,a,j}$, with $a = u,p$ and $j = 1,\ldots,80$, and are plotted in Fig. 3. Once they are substituted in Eqs. (65) and (70) one respectively obtains quantities $\epsilon_u(\alpha_j, r_s)$ and $\epsilon_p(\alpha_j, r_s)$. Finally, the energies per particle in the unpolarized and polarized
case respectively are

$$\epsilon_{\text{wcr},u}(r_s) \equiv \min_{j} \epsilon_u(\alpha_j, r_s)$$  \tag{97}

and

$$\epsilon_{\text{wcr},p}(r_s) \equiv \min_{j} \epsilon_p(\alpha_j, r_s).$$  \tag{98}

The two minimizations also determine the $\alpha$ value associated to a given $r_s$ value in the unpolarized and polarized case. The corresponding $\alpha_u(r_s)$ and $\alpha(r_s)$ functions are plotted in Fig. 3. The quantities $\epsilon_{\text{wcr},u}(r_s)$ and $\epsilon_{\text{wcr},p}(r_s)$ are plotted in Figs. 1 and 2 together with the other approximations mentioned in sect. I. Their comparison with the relevant HF energies shows that the SLQCS approach predicts that the unpolarized and polarized jellium models respectively acquire a simple cubic structure as $r_s$ becomes greater than 90 and 28, and that the stable phase is the polarized one as $r_s > 8.5$. The most recent QMC result\textsuperscript{22} locates the jellium model’s transition from the homogeneous phase to the polarized bcc structure at $r_s = 106 \pm 1$. Further at $r_s = 100$, the energy per particle [in Rydberg] is: -0.0112 by Eq. (3); -0.01448 by the SLQCS approach; -0.014986 by the general HF approach\textsuperscript{30}, -0.01526 by Eq. (9) and -0.0153530(8) by QMC\textsuperscript{22}. These values show that the relevant correlation contributions decrease, i.e. electron interactions are better accounted for, as we go from the first to the last approximation. Moreover, the fact that the values of the second and third approximation are nearly identical indicates that the SLQCS is close to the crystalline HF one, which also predicts a vanishing $n(r)$ on the cell border (see Fig. 5 of Ref.\textsuperscript{22}). A further comparison is possible with the bcc QMC values\textsuperscript{22} at $r_s = 125, 150$ and 200 (in the last case, we consider the energy values resulting from Eq. (12) of Drummond et al.’s). In the three cases the relative errors of the SLQCS values with respect to the QMC ones respectively are: 4.9%, 4.3% and 2.0%. These results show that as the dilution increases the SLQCS more completely accounts for all electron interactions. The reason is probably the following.

The dotted $\alpha_p(r_s)$ curve, reported in Fig.3, shows that the sharpness of the resulting particle density increases as $r_s$ increases and this fact, as explained at the end of the previous section, makes the SLQCS approach more reliable.

VI. CONCLUSIONS

Similarly to the HF analysis of\textsuperscript{30}, this paper provides another application of the Rayleigh-Ritz principle to the Wigner crystal by considering the exact many-body Hamiltonian,
contrast with Wigner’s and Carr’s analyses. To this aim, we considered a class of quantum crystalline states that are essentially determined by the electron density within the unit cell and, by construction, allow no fluctuation in the electron number within each cell. These SLQCSs have the advantage of making the numerical evaluation of the expectation value of the Hamiltonian very simple if one assumes a convenient functional form for the electron density. In this way, one easily obtains an upper bound for the energy of the fundamental state of the jellium model. The comparison of this bound with that obtained by the HF procedure, also based on the variational Rayleigh-Ritz principle, shows that the HF bound is better for the reasons explained in sect. IV. However, the comparison of the SLQCS energies with the HF and the QMC ones shows that the SLQCS values approach to the latter as the density decreases and this indicates that the fluctuations in the electron density within each cell decrease with the density. Finally, the fact the SLQCS approach is a HF one implies that its results can be improved by the perturbative procedure of Moller and Posselt.

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APPENDIX A: ASYMPTOTIC BEHAVIOUR OF $\tilde{G}^2(q, \alpha)$

To show that, as $q \to \infty$, Eq. (96) is the leading asymptotic term of $\tilde{G}^2(q, \alpha)$, defined by Eq. (95), we put

$$g(q, \alpha) \equiv \tilde{G}^2(q, \alpha)/C^2(\alpha) = 2e^{2\alpha}R[e^{-iq}F(q, 2\alpha)]$$  \hspace{1cm} (A1)

with

$$F(q, \alpha) \equiv \int_0^1 e^{iqt - \pi^2(\alpha^2 - t^2)} dt.$$  \hspace{1cm} (A2)

Denoting the above integrand by $f(t, \alpha)$, one sees that $f$ is an analytic function throughout the complex plane $t = u + iv$ deprived of the points 0, 2 and $\infty$. Integral (A2) can be written as

$$i \int_0^a f(i v, \alpha) dv + \int_{i a}^{1+i a} f(u + i a, \alpha) du + i \int_a^0 f(1 + i v, \alpha) dv.$$  \hspace{1cm} (A3)
In the limit $a \to \infty$, one easily verifies that the second integral vanishes because the integral exponentially decreases if $q > 0$. The integrand of the third integral reads

$$e^{iq}e^{-qv-\alpha v^2/(1+v^2)},$$

so that, in the limit $a \to \infty$ one finds

$$-ie^{iq}\int_0^\infty e^{-qv-\alpha v^2/(1+v^2)}dv.$$

This expression, multiplied by $e^{-iq}$ as required by Eq. (A1), is an imaginary quantity and, consequently, it does not contribute to $g(q, \alpha)$. Thus, we find that

$$g(q, \alpha) = 2e^{2\alpha}\Im\left[e^{-iq}\int_0^\infty f_1(v, \alpha)dv\right], \quad \text{(A4)}$$

$$f_1(v, \alpha) \equiv e^{-qv-\alpha/(4+v^2)+i2\alpha/(v(4+v^2))}. \quad \text{(A5)}$$

As $q \to \infty$, the only region $v \approx 0$ contributes to integral (A4), so that the integrand can fairly be approximated by $e^{-\alpha/4+i\alpha/2v}$ and the the asymptotic behaviour of $g(q, \alpha)$ is determined by that of

$$\mathcal{J}(q, \alpha) \equiv \int_0^\infty e^{-qv+i\alpha/2v}dv \quad \text{(A6)}$$

due to the relation

$$g(q, \alpha) \approx 2e^{2\alpha}\Im\left[e^{-iq}e^{-\alpha/4}\mathcal{J}(q, \alpha)\right]. \quad \text{(A7)}$$

Considering the new integration variable $t = v\sqrt{q/2\alpha}$ we find that

$$\frac{x\mathcal{J}_1(x)}{2\alpha} \equiv \frac{\sqrt{q}\mathcal{J}(q, \alpha)}{\sqrt{2\alpha}} = \int_0^\infty e^{-x(t-i/t)}dt = \int_0^\infty e^{-xh(t)}dt \quad \text{(A8)}$$

where we have put $h(t) \equiv (t-i/t)$ and $x \equiv \sqrt{2\alpha q}$. We apply now the saddle point method (see, e.g., Ref. [34]). Thus, we look for the points of the complex plane $t = u + iv$ where the derivative of $h(t)$ vanishes. These points are

$$t_1 = e^{-i\pi/4} = \frac{1-i}{\sqrt{2}} \quad \text{and} \quad t_2 = e^{3i\pi/4} = \frac{-1+i}{\sqrt{2}}. \quad \text{(A9)}$$

The steepest descents through the above two points are determined by the condition $\Im[h(t)] = \text{const}$. In particular, the two steepest descents through $t_1$ respectively have para-
metric equations
\[ u_1(v) = \frac{1 - \sqrt{\Delta(v)}}{2(v + \sqrt{2})}, \quad 0 < v < -1/\sqrt{2}, \quad (A10) \]
\[ u_2(v) = \frac{1 + \sqrt{\Delta(v)}}{2(v + \sqrt{2})}, \quad -1/\sqrt{2} < v < -\sqrt{2}, \quad (A11) \]

with
\[ \Delta(v) \equiv 1 - 8v^2 - 8\sqrt{2}v^3 - 4v^4. \quad (A12) \]

Moreover they form a continuous contour, the first descent going from the origin (when \( v = 0 \)) to \( t_1 \) (when \( v = -1/\sqrt{2} \)) and the second from \( t_1 \) to \( (\infty - i\sqrt{2}) \) (when \( v = -\sqrt{2} \)). Considering the further linear contour joining \( (\infty - i\sqrt{2}) \) to \( (\infty + i0) \), integral (A8) can be written as
\[ \int_{-1/\sqrt{2}}^{0} e^{-x h(u_1(v)+iv)}((u'_1(v) + i)) dv 
+ \int_{-\sqrt{2}}^{-1/\sqrt{2}} e^{-x h(u_2(v)+iv)}((u'_1(v) + i)) dv 
+ i \int_{-\sqrt{2}}^{0} e^{-x h(\infty+iv)} dv. \quad (A13) \]

The last integral vanishes because \( x > 0 \) and \( h(\infty + iv) = \infty \) in the considered integration domain. Further, as \( v \to 0 \) and as \( v \to -\sqrt{2} \) it results that \( \Re[h(u_1(v) + iv)] \to \infty \) and \( \Re[h(u_2(v) + iv)] \to \infty \). Since we are interested in the large \( x \) behaviour, the main contributions to the remaining two integrals in Eq. (A13) arise from the \( v \)-values very close to \(-1/\sqrt{2}\). Expanding \( \Re(h(u_1(v) + iv)) \) and \( \Re(h(u_2(v) + iv)) \) around \( v = -1/\sqrt{2} \) one finds
\[ \Re(h(u_1(v) + iv)) = \Re(h(u_2(v) + iv)) = \sqrt{2} + 2(2 + \sqrt{2})(v + 1/\sqrt{2})^2 + o \]

and integral (A8), equal to Eq. (A13), asymptotically behaves as
\[ (1 + \sqrt{2} - i) \int_{-\infty}^{\infty} e^{-x[(1-i)\sqrt{2}+2(2+\sqrt{2})(v+1/\sqrt{2})^2]} dv = \]
\[ (1 + \sqrt{2} - i) e^{-x(1-i)\sqrt{2}} \sqrt{\frac{\pi}{2x(2 + \sqrt{2})}} e^{-\sqrt{2}x}. \quad (A14) \]

Combining Eqs. (A14), (A8), (A7) and (A1), one finds that the leading asymptotic term of \( \tilde{G}(q, \alpha) \) is that specified by Eq. (96).
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