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Quantum field approach to a low-density electron system

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Abstract. The semiclassical approach to an interacting electron system with low density is replaced by a fully quantum mechanical discussion. The energies of the ground state and the low lying excited states are calculated according to the methods of quantum field theory. A comparison is made with the results of the existing approach. The effect of a magnetic field on the low lying states of the electron system is calculated in a self-consistent way. The low density electron system does not show a Meissner–Ochsenfeld effect.

1. Introduction

The jellium model plays a prominent part in our understanding of the behaviour of the solid state. This model consists of a number of interacting electrons that move against a uniform background of neutralizing positive charge. Up to now its exact solution is unknown and one has to resort to approximation methods in order to study its behaviour. According to Wigner [1], who used a semiclassical approach, the ground state of the jellium model has a lattice structure at sufficiently low densities. This electron lattice is known as the Wigner lattice. For a review of the existing literature on the Wigner lattice we refer to Care and March [2].

The aim of the present article is to discuss the properties of the ground state and the low lying excited states of the low density jellium model from a purely quantum mechanical point of view. Our paper is organized in the following way. First, in section 2, we discuss briefly the formation of a lattice structure in the classical jellium model. Next, in section 3, we give a rather elaborated discussion of the ground state using a quantum field approach. Our calculations are based on the variational method using a Hartree–Fock trial state. Most of the results are familiar, but they are now based on a fully quantum mechanical ground. In section 4 we consider the influence of correlation on the Hartree–Fock results. Section 5 deals with the effect of a magnetic field on the Wigner lattice and pays attention to the eventual appearance of superconductivity. Finally the results are discussed in section 6.

2. Lattice formation in the classical jellium model

First of all we recall briefly the jellium model. The starting-point of our discussion is a system that consists of N electrons and N positive ions moving in a volume Ω.

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The Hamiltonian of this system is given by

$$H = \sum_k \left(\frac{\boldsymbol{p}_k^2}{2m} + \frac{\boldsymbol{\pi}_k^2}{2M} \right) + \tfrac{1}{2} e^2 \sum_{k \neq l} \left(\frac{1}{|\boldsymbol{r}_k - \boldsymbol{r}_l|} + \frac{1}{|\boldsymbol{\rho}_k - \boldsymbol{\rho}_l|} \right) - e^2 \sum_{k,l} \frac{1}{|\boldsymbol{r}_k - \boldsymbol{\rho}_l|} \tag{2.1}$$

where e is the magnitude of the charge of an electron or ion, m the mass of an electron, M the mass of an ion, whereas $\boldsymbol{r}_k$ and $\boldsymbol{p}_k$ denote the position and momentum of electron k and $\boldsymbol{\rho}_k$ and $\boldsymbol{\pi}_k$ those of ion k. Next we use the decomposition

$$\frac{e^2}{r} = \sum_{\boldsymbol{q}} V(\boldsymbol{q}) \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}) \equiv \frac{\Omega}{(2\pi)^3} \int \mathrm{d}^3 q V(\boldsymbol{q}) \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}) \tag{2.2}$$

with

$$V(\boldsymbol{q}) = \frac{1}{\Omega} \int \mathrm{d}^3 r \frac{e^2}{r} \exp(-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}) = \frac{4\pi e^2}{\Omega q^2}. \tag{2.3}$$

It should be remarked here that strictly speaking the expression (2.3) is only true if the Coulomb potential $1/r$ is replaced by the Yukawa potential $e^{-\mu r}/r$ and the limit $\mu \to 0$ is taken after performing the integration. Substitution of (2.2) into (2.1) gives

$$H = \sum_k \left(\frac{\boldsymbol{p}_k^2}{2m} + \frac{\boldsymbol{\pi}_k^2}{2M} \right) + \tfrac{1}{2} \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q}) \Big[\sum_{k \neq l} (\exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)] + \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{\rho}_k - \boldsymbol{\rho}_l)]) - 2 \sum_{k,l} \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{\rho}_l)] \Big] - NV(0) \tag{2.4}$$

where the prime in the summation over $\boldsymbol{q}$ indicates that the $\boldsymbol{q} = 0$ term is excluded. The term $NV(0)$ does not contribute to the energy per electron in the thermodynamic limit, as follows from the integral representation (2.3). Consequently this term can be neglected. The jellium model is then obtained by putting the momenta of the ions equal to zero and by averaging the Hamiltonian (2.4) over all possible configurations of the ions attributing equal weight to them. The result is a homogeneous positively charged background for the electrons. The Hamiltonian of the jellium model is

$$H = \sum_k \frac{\boldsymbol{p}_k^2}{2m} + \tfrac{1}{2} \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q}) \sum_{k \neq l} \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)]. \tag{2.5}$$

Here we pay attention to the energy of the ground state of the classical jellium model. This means that the momenta of the electrons are zero and that we must look for a distribution function $\Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ that minimizes the energy expression

$$E = \tfrac{1}{2} \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q}) \int \mathrm{d}^3 r_1 \ldots \mathrm{d}^3 r_N \Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \sum_{k \neq l} \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)] \tag{2.6}$$

where Φ is normalized, i.e.

$$\int \mathrm{d}^3 r_1 \ldots \mathrm{d}^3 r_N \Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = 1. \tag{2.7}$$

As discussed by Peierls [3] a regular lattice of electrons is expected to be the most stable configuration. Denoting the lattice positions by the set $\{\boldsymbol{R}_k | k = 1, \ldots, N\}$ and putting

$$\Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \prod_{k=1}^{N} \delta^3(\boldsymbol{r}_k - \boldsymbol{R}_k) \tag{2.8}$$

we obtain using (2.3)

$$E = \frac{2\pi e^2}{\Omega} \sum_{\boldsymbol{q}}{}' \sum_{k \neq l} \frac{1}{q^2} \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{R}_k - \boldsymbol{R}_l)]. \tag{2.9}$$

The expression (2.9) contains a summation over the lattice points, which can be easily performed. Then the energy per electron, $\varepsilon = E/N$, appears to be

$$\begin{aligned} \varepsilon &= \frac{2\pi e^2}{N\Omega} \sum_{\boldsymbol{q}}{}' \frac{1}{q^2} \Big(\sum_{k,l} \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{R}_k - \boldsymbol{R}_l)] - N \Big) \\ &= \frac{2\pi e^2}{\Omega} \Big(\sum_{\boldsymbol{K}_n}{}' \frac{N}{K_n^2} - \sum_{\boldsymbol{q}} \sum{}' \frac{1}{q^2} \Big) \end{aligned} \tag{2.10}$$

where $\boldsymbol{K}_n$ denotes a reciprocal lattice vector. The energy ε is negative for all electron densities, as the primitive unit cell of the reciprocal lattice contains N $\boldsymbol{q}$ points. Clearly expression (2.10) consists of two divergent terms. However, their difference is finite as can be shown using the Madelung or Ewald summation procedure. For several lattices the energy ε has been calculated, see e.g. Sholl [4]. It appears that the body-centred cubic lattice has the lowest energy, but it should be remarked here that the energy difference with other simple lattice structures is extremely small.

Summarizing we can conclude that the ground state of the classical jellium model is a BCC lattice for all electron densities.

3. Hartree–Fock ground state of the quantum mechanical low-density jellium model

The Hamiltonian of the quantum mechanical version of the jellium model (2.5) reads in the formalism of second quantization

$$H = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m} c_{k\sigma}^{+} c_{k\sigma} + \tfrac{1}{2} \sum_{\substack{k,k',q \\ \sigma,\sigma'}}{}' V(q) c_{k\sigma}^{+} c_{k'\sigma'}^{+} c_{k'+q\sigma'} c_{k-q\sigma} \tag{3.1}$$

where the fermion operators $c_{k\sigma}^{+}$ and $c_{k\sigma}$ create and annihilate respectively an electron in a plane wave state labeled by the wave vector $\boldsymbol{k}$ and spin σ. The prime in the summation indicates that the $\boldsymbol{q} = 0$ term is excluded because of the presence of the homogeneous positively charged background.

Consider a system consisting of $2N$ electrons, where the number $2N$ has been chosen for convenience. The ground state of the jellium model can be expressed as

$$|\Psi\rangle = \sum_{\sigma_1, \ldots, \sigma_{2N}} \int \mathrm{d}^3 r_1 \ldots \mathrm{d}^3 r_{2N} F(\boldsymbol{r}_1, \sigma_1; \ldots; \boldsymbol{r}_{2N}, \sigma_{2N}) \psi_{\sigma_1}^{+}(\boldsymbol{r}_1) \ldots \psi_{\sigma_{2N}}^{+}(\boldsymbol{r}_{2N}) |\rangle \tag{3.2}$$

where $|\rangle$ denotes the vacuum state and $\psi_\sigma^+(\boldsymbol{r})$ is the usual field operator creating a fermion with spin σ at the position $\boldsymbol{r}$,

$$\psi_\sigma^+(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) c_{\boldsymbol{k}\sigma}^+. \tag{3.3}$$

The function F is determined by the requirement that it must minimize the energy of the system, i.e. the expression

$$E = \langle \Psi | H | \Psi \rangle. \tag{3.4}$$

It should be remarked here that F is not the Schrödinger representation of the ground state of the system. That wavefunction is obtained by constructing the antisymmetrized form of the original function F. The quantity $|F|^2$ plays a similar role as the classical distribution function Φ.

In practice the exact calculation of the ground state energy is still an insurmountable problem. Therefore, one has to resort to approximation methods. Here we have chosen the variational method because of its elegant and insight providing character. In this section we consider the simplest *ansatz* for F, namely the so-called Hartree–Fock (HF) approximation, i.e.

$$F(\boldsymbol{r}_1, \sigma_1; \ldots; \boldsymbol{r}_{2N}, \sigma_{2N}) = C \prod_{n=1}^{2N} f_n(\boldsymbol{r}_n, \sigma_n) \tag{3.5}$$

where the function f_n represents a normalized one-particle wave function, and C is the normalization constant for $|\Psi\rangle$. Next we recall that the ground state of the classical system is a BCC-lattice. Such a structure can also be expected in the quantum mechanical analogue provided that the one-particle wave functions are localized but such that their attendant kinetic energies are small. That requirement can only be fulfilled for an electron system of sufficiently low density. Therefore we restrict ourselves to the low-density jellium model. The translational invariance of the supposed lattice structure implies

$$f_n(\boldsymbol{r}_n, \sigma_n) = f(\boldsymbol{r}_n - \boldsymbol{R}_n)\delta_{\sigma_n \tau_n} \tag{3.6}$$

with $\boldsymbol{R}_n$ being a lattice vector and τ_n the spin of the particle localized at $\boldsymbol{R}_n$. Substitution of (3.5) into (3.2) and making use of (3.6) gives us the following HF trial state as an approximation of the ground state of the low-density jellium model:

$$|\Psi_{\mathrm{HF}}\rangle = C d_{\tau_1}^+(\boldsymbol{R}_1) \ldots d_{\tau_{2N}}^+(\boldsymbol{R}_{2N})|\rangle \tag{3.7}$$

where the operator $d_{\tau_n}^+(\boldsymbol{R}_n)$ describes the creation of an electron with spin τ_n in the wavefunction f localized around the lattice point $\boldsymbol{R}_n$:

$$d_{\tau_n}^+(\boldsymbol{R}_n) = \int \mathrm{d}^3 r \psi_{\tau_n}^+(\boldsymbol{r}) f(\boldsymbol{r} - \boldsymbol{R}_n). \tag{3.8}$$

Representing the wave function as the Fourier integral

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3 k \hat{f}(\boldsymbol{k}) \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \tag{3.9}$$

with

$$\hat{f}(\boldsymbol{k}) = \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3 r f(\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \tag{3.10}$$

the creation operator (3.8) can be expressed as

$$d^+_{\tau_n}(\boldsymbol{R}_n) = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n)\hat{f}(\boldsymbol{k})c^+_{\boldsymbol{k}\tau_n}. \tag{3.11}$$

It follows immediately from (3.8) that the newly defined creation and annihilation operators satisfy the following anticommutation relations

$$\begin{aligned} &\{d_{\tau_m}(\boldsymbol{R}_m), d^+_{\tau_n}(\boldsymbol{R}_n)\} = \delta_{\tau_m\tau_n} S(\boldsymbol{R}_m - \boldsymbol{R}_n) \\ &\{d_{\tau_m}(\boldsymbol{R}_m), d_{\tau_n}(\boldsymbol{R}_n)\} = \{d^+_{\tau_m}(\boldsymbol{R}_m), d^+_{\tau_n}(\boldsymbol{R}_n)\} = 0 \end{aligned} \tag{3.12}$$

where

$$S(\boldsymbol{R}_m - \boldsymbol{R}_n) = \int \mathrm{d}^3 r f^*(\boldsymbol{r} - \boldsymbol{R}_m) f(\boldsymbol{r} - \boldsymbol{R}_n). \tag{3.13}$$

The quantity $S(\boldsymbol{R}_m - \boldsymbol{R}_n)$ is the overlap of two wavefunctions centred around $\boldsymbol{R}_m$ and $\boldsymbol{R}_n$ respectively.

In a first approximation the overlap between the distinct wavefunctions can be neglected. Then the energy appears to be independent of the spin configuration as shown in appendix 1. The resulting energy, which is a functional of the wavefunction f, is just the Hartree energy

$$E_{\mathrm{H}}(f) = 2N \int \mathrm{d}^3 k \frac{\hbar^2 k^2}{2m} \hat{f}(\boldsymbol{k})\hat{f}^*(\boldsymbol{k}) + \tfrac{1}{2} \sum_{\boldsymbol{q}}{}' \sum_{m\neq n} \tilde{V}(\boldsymbol{q}) \exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_n - \boldsymbol{R}_m)] \tag{3.14}$$

where

$$\tilde{V}(\boldsymbol{q}) = V(\boldsymbol{q}) \left[\int \mathrm{d}^3 k \hat{f}(\boldsymbol{k}+\boldsymbol{q})\hat{f}^*(\boldsymbol{k})\right]^2. \tag{3.15}$$

Note: it should be stressed here that the expression for the Hartree energy still contains terms of the order of the overlap. These terms do not originate from the presence of $S(\boldsymbol{R}_m - \boldsymbol{R}_n)$ in the anticommutation relations (3.12) but are due to the form of $\tilde{V}(\boldsymbol{q})$ given by (3.15). Clearly $\tilde{V}(\boldsymbol{q})$ is not the Fourier transform of the Coulomb potential but of some smeared-out potential that depends on the wavefunction f itself.

The explicit form of the wavefunction f follows from the condition that f must minimize $E_{\mathrm{H}}(f)$. That minimization procedure is discussed in appendix 2. It appears that the resulting form is given by

$$f_0(\boldsymbol{r}) = \frac{1}{(2\alpha\pi)^{3/4}} \exp\left(-\frac{r^2}{4\alpha}\right) \tag{3.16}$$

with

$$\alpha^2 = \frac{3\Omega}{32\pi N}\frac{\hbar^2}{me^2} \tag{3.17}$$

provided that all terms of the order of the overlap are neglected. The attendant Hartree energy is

$$E_H^{(0)} = E_{Cl} + 2N\frac{8\pi N e^2 \alpha}{\Omega} \tag{3.18}$$

where E_{Cl} denotes the energy of the classical electron lattice. We like to remark here that $E_H^{(0)}$ is not the energy obtained by substituting (3.16) into (3.14), the difference being of the order of the overlap.

In order to compare our results with existing ones we use the Bohr unit $a_0 = \hbar^2/me^2$ as the unit of length and the Rydberg, which equals $e^2/2a_0$, as the unit of energy. Further we express the electron density ρ in terms of the dimensionless parameter r_s according to:

$$\rho = \frac{2N}{\Omega} = \left(\tfrac{4}{3}\pi r_s^3 a_0^3\right)^{-1}. \tag{3.19}$$

Then the following expressions are obtained for α and $E_H^{(0)}$ respectively:

$$\alpha = \tfrac{1}{2} r_s^{3/2} a_0^2 \tag{3.20}$$

$$E_H^{(0)} = 2N\left(-\frac{A}{r_s} + \frac{3}{r_s^{3/2}}\right) \tag{3.21}$$

where A is the Madelung constant of the classical electron lattice.

The overlap (3.13) can be easily calculated for a wavefunction of the form (3.16) and appears to be

$$S(\boldsymbol{R}_{mn}) = \exp\left(-\frac{R_{mn}^2}{8\alpha}\right) = \exp\left(-\tfrac{1}{4}\tilde{R}_{mn}^2 r_s^{1/2}\right) \tag{3.22}$$

with $|\boldsymbol{R}_m - \boldsymbol{R}_n| = |\boldsymbol{R}_{mn}| = R_{mn}$ and $\tilde{R}_{mn} = R_{mn}/r_s a_0$, i.e. $\tilde{R}_{mn}$ is a dimensionless measure for the distance between the lattice positions $\boldsymbol{R}_m$ and $\boldsymbol{R}_n$. The quantity $\tilde{R}_{mn}$ is of the order of one or larger as the lattice distance is of the order of $r_s a_0$. Consequently the overlap is very small indeed at low density, i.e. for large r_s.

Our results (3.20) and (3.21) are exactly equal to those of Wigner, i.e. the Wigner treatment is equivalent to an approximate Hartree–Fock calculation based on localized one-electron wavefunctions. The approximation consists of neglecting the mutual overlap (3.22) of the wavefunctions in the anticommutation relations (3.12) plus all terms in the resulting Hartree energy, which are of the same order as the overlap.

The difference between the Hartree–Fock energy and the Hartree energy is known as the exchange energy and depends on the spin configuration of the underlying lattice. In the following we discuss the Hartree–Fock energy up to order $S(\boldsymbol{R}_{mn})^2$ for both the ferromagnetic and the antiferromagnetic spin configuration. The overlap terms of order $S(\boldsymbol{R}_{mn})^2$ are two-particle exchange terms. These terms have also

been discussed by Carr [5]. Higher order corrections to the Wigner energy (3.21) are not considered here because of the complexity of the calculations.

As shown in appendix 2 the wavefunction, that minimizes the Hartree–Fock energy E_{HF} up to order $S(\boldsymbol{R}_{mn})^2$, is given by (3.16) plus correction terms of order $S(\boldsymbol{R}_{mn})^2$. The effect of these last terms on E_{HF}, however, is of order $S(\boldsymbol{R}_{mn})^4$ and can therefore be neglected. Thus E_{HF} can be calculated exactly up to order $S(\boldsymbol{R}_{mn})^2$, using the wavefunction (3.16) with the Wigner α (3.17). The effect of the overlap on the wavefunction itself is extremely difficult to calculate even up to order $S(\boldsymbol{R}_{mn})^2$. However, that effect can be estimated by choosing the wave function (3.16) as a trial function with variational parameter α and subsequently minimizing the expression for the Hartree–Fock energy up to order $S(\boldsymbol{R}_{mn})^2$ with respect to α. The difference between the resulting value of α and the Wigner value (3.17) is then a measure for the influence of exchange on the wavefunction.

Up to order $S(\boldsymbol{R}_{mn})^2$ the Hartree–Fock energy consists of two terms. The first term is obtained by substituting (3.16) into (3.14) and performing the lattice sum. It is the total Hartree energy, including all terms of order $S(\boldsymbol{R}_{mn})^2$. The second term is the two-particle exchange energy ΔE_{HF}. The calculation of this energy is given in appendix 1. Thus the Hartree–Fock energy can be expressed as

$$E_{HF} = 2N\left[\frac{3\hbar^2}{8m\alpha} + N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n) - \tfrac{1}{2}\sum_{\boldsymbol{q}}{}'\tilde{V}(\boldsymbol{q})\right] + \Delta E_{HF} \tag{3.23}$$

where

$$\tilde{V}(\boldsymbol{q}) = \frac{4\pi e^2}{\Omega q^2}\exp(-\alpha q^2) \tag{3.24}$$

and the summation over $\boldsymbol{K}_n$ $(n = 1,2,\ldots,2N)$ runs over the reciprocal lattice vectors. The contribution ΔE_{HF} depends on the spin configuration of the Wigner lattice. Here we consider both the purely ferromagnetic configuration and an antiferromagnetic configuration consisting of two interpenetrating sublattices having an oppositely directed purely ferromagnetic spin configuration.

The ferromagnetic two-particle exchange energy is given in expression (A1.24) of appendix 1. After performing a simple lattice summation we find

$$\Delta E_{HF}^{f} = 2N\sum_{\boldsymbol{R}_n\neq 0} e^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + 2N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n)\left[1 - e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}\right]\right.$$
$$\left. + \sum_{\boldsymbol{q}}{}'\tilde{V}(\boldsymbol{q})\left[2e^{\frac{1}{2}i\boldsymbol{q}\cdot\boldsymbol{R}_n} - \tfrac{3}{2} - \tfrac{1}{2}e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}\right]\right] \tag{3.25}$$

where the summation over $\boldsymbol{R}_n$ ($n = 1,2,\ldots,2N$) runs over the sites of the Wigner lattice, whose reciprocal lattice vectors are denoted by $\boldsymbol{K}_n$. The antiferromagnetic contribution, which is given in (A1.25) is found to read, after performing a simple lattice summation

$$\Delta E_{HF}^{a} = 2N\sum_{\boldsymbol{R}_n\neq 0} e^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n)[1 + e^{i\boldsymbol{K}_n\cdot\boldsymbol{\delta}}][1 - e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}]\right.$$
$$\left. + \sum_{\boldsymbol{q}}{}'\tilde{V}(\boldsymbol{q})[2e^{\frac{1}{2}i\boldsymbol{q}\cdot\boldsymbol{R}_n} - \tfrac{3}{2} - \tfrac{1}{2}e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}]\right] \tag{3.26}$$

where the summations over $\boldsymbol{R}_n$ and $\boldsymbol{K}_n$ ($n = 1, 2, \ldots, N$) now run over the sites of the ferromagnetic sublattice and its reciprocal lattice vectors respectively. The vector δ describes the position of both sublattices with respect to each other.

For an explicit calculation of the quantities given by (3.23), (3.25) and (3.26) we use the Ewald summation method and replace the Riemann sum over q by an integration. Then we obtain the following expression for the Hartree–Fock energy (see appendix 3):

$$E_{\mathrm{HF}} = 2N\left[\frac{3\hbar^2}{8m\alpha} + \frac{4\pi Ne^2}{\Omega}(\alpha-\beta) + \frac{4\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{\mathrm{e}^{-\beta K_n^2}}{K_n^2} - \frac{e^2}{2\sqrt{\pi\beta}} + \tfrac{1}{2}e^2\sum_{\boldsymbol{R}_n\neq 0}\frac{1}{R_n}\left[\operatorname{erfc}\left(\frac{R_n}{2\sqrt{\beta}}\right) - \operatorname{erfc}\left(\frac{R_n}{2\sqrt{\alpha}}\right)\right]\right] + \Delta E_{\mathrm{HF}} \tag{3.27}$$

where β is the Ewald parameter and $\operatorname{erfc}(x)$ is the complement of the error function $\operatorname{erf}(x)$. The ferromagnetic and antiferromagnetic two-particle exchange contributions are respectively given by

$$\Delta E^{\mathrm{f}}_{\mathrm{HF}} = 2N\sum_{\boldsymbol{R}_n\neq 0}\mathrm{e}^{-R_n^2/4\alpha}\left[\frac{\hbar^2R_n^2}{32m\alpha^2} - \frac{3e^2}{2\sqrt{\pi\alpha}} - \frac{e^2}{2R_n}\operatorname{erf}\left(\frac{R_n}{2\sqrt{\alpha}}\right) + \frac{4e^2}{R_n}\operatorname{erf}\left(\frac{R_n}{4\sqrt{\alpha}}\right) + \frac{8\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{\mathrm{e}^{-\beta K_n^2}}{K_n^2}[1-\mathrm{e}^{-\frac{1}{2}\mathrm{i}\boldsymbol{K}_n\cdot\boldsymbol{R}_n}] + e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}\left[\operatorname{erfc}\left(\frac{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\alpha}}\right) - \operatorname{erfc}\left(\frac{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\beta}}\right)\right] + e^2\sum_{\boldsymbol{R}_m}\frac{1}{R_m}\left[\operatorname{erfc}\left(\frac{R_m}{2\sqrt{\beta}}\right) - \operatorname{erfc}\left(\frac{R_m}{2\sqrt{\alpha}}\right)\right]\right] \tag{3.28}$$

and

$$\Delta E^{\mathrm{a}}_{\mathrm{HF}} = 2N\sum_{\boldsymbol{R}_n}\mathrm{e}^{-R_n^2/4\alpha}\left[\frac{\hbar^2R_n^2}{32m\alpha^2} - \frac{3e^2}{2\sqrt{\pi\alpha}} - \frac{e^2}{2R_n}\operatorname{erf}\left(\frac{R_n}{2\sqrt{\alpha}}\right) + \frac{4e^2}{R_n}\operatorname{erf}\left(\frac{R_n}{4\sqrt{\alpha}}\right) + \sum_{\boldsymbol{a}=0,\delta}\left\{\frac{4\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{\mathrm{e}^{-\beta K_n^2}}{K_n^2}\mathrm{e}^{\mathrm{i}\boldsymbol{K}_n\cdot\boldsymbol{a}}[1-\mathrm{e}^{-\frac{1}{2}\mathrm{i}\boldsymbol{K}_n\cdot\boldsymbol{R}_n}] + e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}\left[\operatorname{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\alpha}}\right) - \operatorname{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\beta}}\right)\right] + e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m+\boldsymbol{a}|}\left[\operatorname{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}|}{2\sqrt{\beta}}\right) - \operatorname{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}|}{2\sqrt{\alpha}}\right)\right]\right\}\right]. \tag{3.29}$$

It should be remarked here that E_{HF} does not depend on β. The sole reason for introducing this parameter is to achieve a rapid convergence of the appearing sums over the reciprocal lattice vectors. Next we introduce the dimensionless quantities

$$\tilde{\alpha} = \frac{\alpha}{a_0^2} \qquad \tilde{\beta} = \frac{\beta}{r_s^2a_0^2} \qquad \tilde{\boldsymbol{R}}_n = \frac{\boldsymbol{R}_n}{r_sa_0} \qquad \tilde{\boldsymbol{K}}_n = r_sa_0 \qquad \boldsymbol{K}_n\tilde{\delta} = \frac{\delta}{r_sa_0}.$$

Then the Hartree–Fock energy can be expressed in Rydberg units reading

$$E_{\mathrm{HF}} = 2N\left[\frac{-A}{r_s} + \frac{3}{4\tilde{\alpha}} + \frac{3\tilde{\alpha}}{r_s^3} - \frac{1}{r_s}\sum_{\tilde{R}_n\neq 0}\frac{1}{\tilde{R}_n}\mathrm{erfc}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}}\right)\right] + \Delta E_{\mathrm{HF}} \tag{3.30}$$

where the Madelung constant A is given by

$$A = \frac{1}{\sqrt{\pi\tilde{\beta}}} + 3\tilde{\beta} - 3\sum_{\tilde{K}_n\neq 0}\frac{1}{\tilde{K}_n^2}\mathrm{e}^{-\tilde{\beta}\tilde{K}_n^2} - \sum_{\tilde{R}_n\neq 0}\frac{1}{\tilde{R}_n}\mathrm{erfc}\left(\frac{\tilde{R}_n}{2\sqrt{\tilde{\beta}}}\right). \tag{3.31}$$

The relevant two-particle exchange contributions are given by

$$\begin{aligned}\Delta E_{\mathrm{HF}}^{\mathrm{f}} = 2N\sum_{\tilde{R}_n\neq 0}\mathrm{e}^{-\tilde{R}_n^2 r_s^2/4\tilde{\alpha}}&\left[\frac{\tilde{R}_n^2 r_s^2}{16\tilde{\alpha}^2} - \frac{3}{\sqrt{\pi\tilde{\alpha}}} + \frac{8}{\tilde{R}_n r_s}\mathrm{erf}\left(\frac{\tilde{R}_n r_s}{4\sqrt{\tilde{\alpha}}}\right)\right.\\
&- \frac{1}{\tilde{R}_n r_s}\mathrm{erf}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}}\right) + \frac{6}{r_s}\sum_{\tilde{K}_n\neq 0}\frac{1}{\tilde{K}_n^2}\mathrm{e}^{-\tilde{\beta}\tilde{K}_n^2}[1-\mathrm{e}^{-\frac{1}{2}\mathrm{i}\tilde{K}_n\cdot\tilde{R}_n}]\\
&+ \frac{2}{r_s}\sum_{\tilde{R}_m}\frac{1}{|\tilde{R}_m - \frac{1}{2}\tilde{R}_n|}\left[\mathrm{erfc}\left(\frac{|\tilde{R}_m - \frac{1}{2}\tilde{R}_n| r_s}{2\sqrt{\tilde{\alpha}}}\right) - \mathrm{erfc}\left(\frac{|\tilde{R}_m - \frac{1}{2}\tilde{R}_n|}{2\sqrt{\tilde{\beta}}}\right)\right]\\
&\left.+ \frac{2}{r_s}\sum_{\tilde{R}_m}\frac{1}{\tilde{R}_m}\left[\mathrm{erfc}\left(\frac{\tilde{R}_m}{2\sqrt{\tilde{\beta}}}\right) - \mathrm{erfc}\left(\frac{\tilde{R}_m r_s}{2\sqrt{\tilde{\alpha}}}\right)\right]\right]\end{aligned} \tag{3.32}$$

and

$$\begin{aligned}\Delta E_{\mathrm{HF}}^{\mathrm{a}} = 2N\sum_{\tilde{R}_n\neq 0}\mathrm{e}^{-\tilde{R}_n^2 r_s^2/4\tilde{\alpha}}&\left[\frac{\tilde{R}_n^2 r_s^2}{16\tilde{\alpha}^2} - \frac{3}{\sqrt{\pi\tilde{\alpha}}} + \frac{8}{\tilde{R}_n r_s}\mathrm{erf}\left(\frac{\tilde{R}_n r_s}{4\sqrt{\tilde{\alpha}}}\right) - \frac{1}{\tilde{R}_n r_s}\mathrm{erf}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}}\right)\right.\\
&+ \sum_{\tilde{a}=0,\tilde{\delta}}\left\{\frac{3}{r_s}\sum_{\tilde{K}_n\neq 0}\frac{1}{\tilde{K}_n^2}\mathrm{e}^{-\tilde{\beta}\tilde{K}_n^2}\mathrm{e}^{\mathrm{i}\tilde{K}_n\cdot\tilde{a}}[1-\mathrm{e}^{-\frac{1}{2}\mathrm{i}\tilde{K}_n\cdot\tilde{R}_n}]\right.\\
&+ \frac{2}{r_s}\sum_{\tilde{R}_m}\frac{1}{|\tilde{R}_m + \tilde{a} - \frac{1}{2}\tilde{R}_n|}\left[\mathrm{erfc}\left(\frac{|\tilde{R}_m + \tilde{a} - \frac{1}{2}\tilde{R}_n| r_s}{2\sqrt{\tilde{\alpha}}}\right)\right.\\
&\left.- \mathrm{erfc}\left(\frac{|\tilde{R}_m + \tilde{a} - \frac{1}{2}\tilde{R}_n|}{2\sqrt{\tilde{\beta}}}\right)\right]\\
&\left.\left.+ \frac{2}{r_s}\sum_{\tilde{R}_m}\frac{1}{|\tilde{R}_m + \tilde{a}|}\left[\mathrm{erfc}\left(\frac{|\tilde{R}_m + \tilde{a}|}{2\sqrt{\tilde{\beta}}}\right) - \mathrm{erfc}\left(\frac{|\tilde{R}_m + \tilde{a}| r_s}{2\sqrt{\tilde{\alpha}}}\right)\right]\right\}\right].\end{aligned} \tag{3.33}$$

The quantities given by (3.30), (3.31), (3.32) and (3.33) must be calculated numerically. In order to check our computer program we recalculated the Madelung constants of four simple lattice structures. Our results are exactly those of Sholl [4] and are reproduced in table I for convenience' sake. It should be mentioned here that

Table 1. Madelung constants of four simple lattice structures.

Lattice structure	Madelung constant A
SC	1.76012
FCC	1.79175
HCP	1.79168
BCC	1.79186

the expression (3.31) cannot be used for the calculation of the Madelung constant of the hcp-lattice, as the attendant unit cell contains two electrons. Instead one has to start from expression (3.14) with N electrons at the lattice sites $\boldsymbol{R}_n$ of the unit cells and N electrons at the positions $\boldsymbol{R}_n + \delta$, where δ denotes the position of the electron inside the unit cell.

The exact value of E_{HF} up to order $S(\boldsymbol{R}_{mn})^2$ was obtained by substituting the Wigner value $\tilde{\alpha} = \frac{1}{2}r_s^{3/2}$ into (3.30), (3.32) and (3.33). As is usual we took as a measure for the stability of the lattice the energy difference between the Hartree–Fock energy E_{HF} of the Wigner lattice and the Hartree–Fock energy E_0 of the free electron gas. The energy E_0 in Rydbergs is given by [6]

$$E_0 = 2N\left(\frac{2.2099}{r_s^2} - \frac{0.9163}{r_s}\right). \tag{3.34}$$

In figure 1 this energy difference per electron, $\epsilon = 1/2N(E_{\mathrm{HF}} - E_0)$, is shown for all simple ferromagnetic and antiferromagnetic lattice structures.

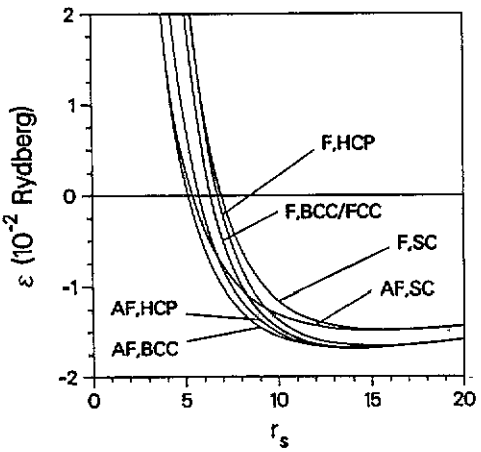

Figure 1. Energy difference per electron, ϵ, between the Hartree–Fock energy of the Wigner lattice and that of the free electron gas plotted as a function of r_s for the simple ferromagnetic (F) and antiferromagnetic (AF) lattice structures.

In order to demonstrate the influence of the two-particle exchange contributions on the width of the one-particle wavefunction the value of the variational parameter $\tilde{\alpha}$ was obtained numerically by minimizing E_{HF} with respect to $\tilde{\alpha}$ using an iteration procedure that starts from the Wigner value. In figure 2 the resulting $\tilde{\alpha}$ is shown as a function of r_s for a ferromagnetic BCC-lattice. Here the r_s-dependence of

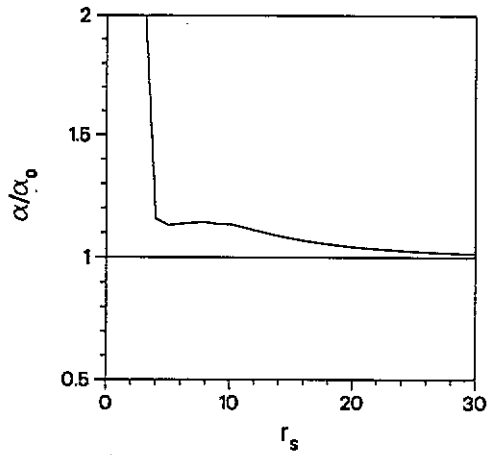

Figure 2. Square of the width of the one-particle wavefunction, α, given as a function of r_s in units of the Wigner value $\alpha_0 = \frac{1}{2}r_s^{3/2}a_0^2$ for the ferromagnetic BCC-lattice.

the Wigner $\tilde{\alpha}$ is represented as well. It appears that the other ferromagnetic and antiferromagnetic lattices give practically the same r_s-dependence of $\tilde{\alpha}$.

Summarizing, the results of the present Hartree–Fock calculations are as follows:

(i) In contrast with the classical electron system the ground state of the quantum mechanical system is a Wigner lattice only at low densities. In the case of a BCC-lattice we find that $\varepsilon = 0$ at $r_s \simeq 5$, i.e. the proposed lattice structure is not stable for higher densities.

(ii) The two-particle exchange contributions remove the degeneracy of the ground state with respect to all possible spin configurations of the lattice. The antiferromagnetic structure is stable compared with the ferromagnetic structure in the range $5 \leqslant r_s \leqslant 14$, the ferromagnetic structure has the lowest energy at lower densities, $r_s > 14$. In that region, however, the energy difference between both structures is extremely small. Consequently a small inaccuracy in the calculation of the two-particle exchange contributions can produce a large error in the critical value of r_s where both lattices have equal energy. As is shown in appendix 4 this accounts for the discrepancy between our critical value $r_s = 14$ and Carr's result $r_s = 270$ [5].

(iii) The exchange influences the width of the localized one-electron wavefunctions. It appears that the width increases with respect to the Wigner value, i.e. the wave packets become less localized.

4. Correlation in the Wigner lattice

The effect of correlation on the HF ground state energy has been discussed by Carr [5]. He replaced the original Wigner lattice of uncoupled oscillators by a lattice of coupled oscillators. The semiclassical nature of his approach, however, raises some epistemological questions. In order to discuss these questions properly we first summarize Carr's approach.

By analogy with Born's lattice theory [7] Carr expanded the electron–electron interaction around the equilibrium positions $\boldsymbol{R}_i$ of the electrons. These positions are

thought to form a lattice. The expansion in terms of the displacements $r_i - R_i$ gives rise to the following Hamiltonian for the electron system:

$$H = E_{\mathrm{Cl}} + \sum_i \frac{p_i^2}{2m} + \tfrac{1}{2}\sum_{i\neq j}(r_i - R_i)M(R_{ij})(r_j - R_j) + \dots \qquad (4.1)$$

where E_{Cl} denotes the Madelung energy of the classical electron lattice. The elements $M(R_{ij})_{\mu\nu}$, with $\mu, \nu = x, y, z$, of the second rank tensor $M(R_{ij})$ are given by

$$M(R_{ij})_{\mu\nu} = \frac{\partial^2}{\partial R_i^\mu \partial R_j^\nu}\left(\frac{e^2}{|R_i - R_j|}\right) \qquad i \neq j$$
$$M(0)_{\mu\nu} = \frac{8\pi N e^2}{3\Omega}\delta_{\mu\nu}. \qquad (4.2)$$

Neglecting the anharmonic terms in the expansion (4.1) the remaining problem was solved in the familiar way by introducing the normal coordinates

$$q_{k\lambda} = \frac{1}{\sqrt{2N}}\sum_i e^{ik\cdot R_i}\varepsilon_{k\lambda}\cdot(r_i - R_i)$$
$$p_{k\lambda} = \frac{1}{\sqrt{2N}}\sum_i e^{ik\cdot R_i}\varepsilon_{k\lambda}\cdot p_i \qquad (4.3)$$

with $2N$ denoting the number of electrons and k and λ being the wave vector and polarization index ($\lambda = 1, 2, 3$) of the vibrational eigenmodes, respectively. The polarization vectors $\varepsilon_{k\lambda}$ are determined by the eigenvalue equation

$$\sum_i e^{ik\cdot R_{ij}} M(R_{ij})\varepsilon_{k\lambda} = m\omega_{k\lambda}^2 \varepsilon_{k\lambda} \qquad (4.4)$$

where $\omega_{k\lambda}$ is the frequency of an eigenmode. Next the quantum nature of the system was taken into account by requiring $[q_{k\lambda}, p_{k'\lambda'}] = i\hbar\delta_{kk'}\delta_{\lambda\lambda'}$. Introducing the boson operators

$$a_{k\lambda}^+ = [2\hbar m\omega_{k\lambda}]^{-1/2}[m\omega_{k\lambda}q_{-k\lambda} - ip_{k\lambda}]$$
$$a_{k\lambda} = [2\hbar m\omega_{k\lambda}]^{-1/2}[m\omega_{k\lambda}q_{k\lambda} + ip_{-k\lambda}] \qquad (4.5)$$

the following Hamiltonian resulted for the low density electron system:

$$H_C = E_{\mathrm{Cl}} + \sum_{k\lambda}\hbar\omega_{k\lambda}\left[\tfrac{1}{2} + a_{k\lambda}^+ a_{k\lambda}\right]. \qquad (4.6)$$

After calculating the eigenfrequencies from (4.4) and performing the sum over k and λ by using a numerical integration procedure Carr arrived at a ground state energy in Rydberg units given by

$$E_C^{(0)} = 2N\left(\frac{-A}{r_s} + \frac{2.66}{r_s^{3/2}}\right) = E_{\mathrm{H}}^{(0)} - 2N\frac{0.34}{r_s^{3/2}} \qquad (4.7)$$

where $E_H^{(0)}$ is the Wigner ground state energy (3.21).

The ground state $|\varphi_{\text{harm}}\rangle$ that belongs to the energy (4.7), is found by the requirement

$$a_{k\lambda}|\varphi_{\text{harm}}\rangle = 0 \tag{4.8}$$

for all k and λ. In coordinate-language this ground state is represented by the wavefunction

$$\begin{aligned}\varphi_{\text{harm}}(r_1,\ldots,r_{2N}) &= \prod_{k,\lambda}\left(\frac{m\omega_{k\lambda}}{\pi k}\right)^{1/4}\exp\left[-\frac{m\omega_{k\lambda}}{2\hbar}q_{k\lambda}(r_1,\ldots,r_{2N})q_{-k\lambda}(r_1,\ldots,r_{2N})\right]\\ &= \exp\left[-\sum_{i\neq j}u_{ij}(r_i,r_j)\right]\prod_{i=1}^{2N}f(r_i-R_i)\end{aligned} \tag{4.9}$$

where the functions f and u_{ij} are given by, respectively,

$$\begin{aligned}f(r_i-R_i) &= \left[\prod_{k\lambda}\left(\frac{m\omega_{k\lambda}}{2\hbar}\right)\right]^{1/2N}\\ &\quad\times\exp\left[\frac{-1}{2N}\sum_{k\lambda}\left(\frac{m\omega_{k\lambda}}{2\hbar}\right)[(r_i-R_i)\cdot\varepsilon_{k\lambda}][\varepsilon_{-k\lambda}\cdot(r_i-R_i)]\right]\\ u_{ij}(r_i,r_j) &= \frac{1}{2N}\sum_{k\lambda}\left(\frac{m\omega_{k\lambda}}{2\hbar}\right)e^{ik\cdot R_{ij}}[(r_i-R_i)\cdot\varepsilon_{k\lambda}][\varepsilon_{-k\lambda}\cdot(r_j-R_j)].\end{aligned} \tag{4.10}$$

Clearly $\varphi_{\text{harm}}(r_1,\ldots,r_{2N})$ is not antisymmetric in the coordinates of the electrons, i.e. this wavefunction cannot describe the ground state of the low density electron system as the effect of exchange is excluded. In order to estimate *a posteriori* the magnitude of this neglected contribution to the ground state energy Carr calculated, starting from a basis set of Slater determinants of harmonic oscillator wave functions, the matrix elements of the total Hamiltonian. It appeared that the exchange terms fell off like $\exp(-Cr_s^{1/2})$, where C is some constant. Therefore he concluded that the expansion of the Hamiltonian (4.1) leads to exact results provided that all these exponential terms can be neglected. Then the expression (4.7) for the ground state energy of the low density electron system is exact up to order $r_s^{-3/2}$.

In our opinion Carr's result (4.7) for the ground state energy is correct, but his approach raises the following epistemological questions.

(i) The Hamiltonian, which is obtained after breaking off the expansion (4.1), is no longer invariant under the permutation of the coordinates of the electrons. This means that the electrons are conceived as distinguishable particles, i.e. Carr's approach violates an important quantum mechanical principle. The resulting system of distinguishable electrons vibrating around their equilibrium positions is then considered as a quantum system and dealt with accordingly. The question is now whether it is possible to derive Carr's result in a fully quantum mechanical way, i.e. without violating the permutation symmetry.

(ii) Carr describes the electrons in terms of boson operators known as phonons. The introduction of the phonon concept, however, is only a mathematical convenience. Consequently a well-defined relation between the boson operators (4.5) and the original fermion operators describing the creation and annihilation of electrons must exist. What is the form of that relation?

(iii) The semiclassical approach of Carr does not lead to an antisymmetric ground state wave function with the energy as given in (4.7). According to Carr that wavefunction can in principle be calculated *a posteriori* by diagonalizing the Hamiltonian matrix that is obtained from the complete set of Slater determinants of harmonic oscillator wavefunctions, which are the solutions of (4.6). However Carr does not give an algorithm needed to actually perform this calculation. It seems plausible that the antisymmetric wavefunction based upon (4.9), i.e.

$$|\varphi^{A}_{\text{harm}}\rangle = \int \mathrm{d}^3 r_1 \ldots \mathrm{d}^3 r_{2N} \varphi_{\text{harm}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{2N}) \psi^{+}_{\tau_1}(\boldsymbol{r}_1) \ldots \psi^{+}_{\tau_{2N}}(\boldsymbol{r}_{2N}) |\rangle \tag{4.11}$$

might possibly lead to the required energy (4.7), provided that all exponential terms appearing in the energy expression are neglected. It should be remarked, however, that such a suggestion is still unfounded. Obviously a fully quantum mechanical approach leads in principle directly to an antisymmetric ground state wavefunction. The question is then how to obtain that wavefunction.

A possible way to answer the posed questions is to use the variational method starting with an *ansatz* of the form (4.11) for the wavefunction. That would be a logical continuation of the approach discussed in section 3. Unfortunately, such an *ansatz* is too complicated in the present case. In fact any variational calculation, that is based upon an *ansatz* for a many-electron wavefunction unlike the Hartree–Fock type, is extremely difficult. Therefore another method must be looked for, that should preferably reproduce the original Wigner result as well. Here we introduce a fully quantum mechanical approach, which is partly based on work by Brenig [8], Fredkin and Werthamer [9] and Pietrass [10].

The starting point of the present approach is to represent the eigenstates of the low density electron system as linear combinations of Slater determinants of one-electron states. Such a decomposition is always possible provided that these one-electron states form a complete set. In view of the results already obtained in section 3 the set of eigenstates of the harmonic oscillator is an obvious choice. The important consequence of this choice is that the decompositions of the system's ground state and low lying excited states involve only a limited number of important terms, namely those terms that contain the ground state and the low lying states of the harmonic oscillator. In terms of the Cartesian coordinates x, y, z the harmonic oscillator eigenfunctions are given by

$$f_{\boldsymbol{\jmath}}(\boldsymbol{r}) = \prod_{\hat{\boldsymbol{\xi}}} [\sqrt{2\alpha\pi} 2^{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}} (\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})!]^{-1/2} \exp\left[\frac{-(\boldsymbol{r}\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right] H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}\left(\frac{\boldsymbol{r}\cdot\hat{\boldsymbol{\xi}}}{\sqrt{2\alpha}}\right) \tag{4.12}$$

where $\hat{\boldsymbol{\xi}}$ runs over the basis vectors, $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$ of a given Cartesian coordinate system, $\boldsymbol{\jmath} = (j_x, j_y, j_z)$, $\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}} = 0, 1, 2, \ldots$, and $H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}$ is the Hermite polynomial of order $\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}$. The width $\alpha^{1/2}$ of the functions $f_{\boldsymbol{\jmath}}$ is still arbitrary. In terms of the given one-electron functions the eigenstates $|\psi_n\rangle$ of a low density electron system

consisting of $2N$ electrons can be expressed as (cf (3.7))

$$|\psi_n\rangle = \sum_{\substack{\mathfrak{z}_1,\mathfrak{z}_2,\ldots,\mathfrak{z}_{2N} \\ \sigma_1,\sigma_2,\ldots,\sigma_{2N}}} A^{\sigma_1\ldots\sigma_{2N}}_{\mathfrak{z}_1\ldots\mathfrak{z}_{2N}}(n) d^+_{\mathfrak{z}_1\sigma_1}(\boldsymbol{R}_1)\ldots d^+_{\mathfrak{z}_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle \quad (4.13)$$

where the operator $d^+_{\mathfrak{z}_i\sigma_i}(\boldsymbol{R}_i)$ describes the creation of an electron with spin σ_i in the harmonic oscillator eigenfunction $f_{\mathfrak{z}_i}$ localized around lattice site $\boldsymbol{R}_i$:

$$d^+_{\mathfrak{z}_i\sigma_i}(\boldsymbol{R}_i) = \int \mathrm{d}^3 r \psi^+_{\sigma_i}(\boldsymbol{r}) f_{\mathfrak{z}_i}(\boldsymbol{r}-\boldsymbol{R}_i) = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{f}_{\mathfrak{z}_i}(\boldsymbol{k}) c^+_{\boldsymbol{k}\sigma_i} \quad (4.14)$$

with $\hat{f}_{\mathfrak{z}_i}$ being the Fourier transform of $f_{\mathfrak{z}_i}$, i.e.

$$\begin{aligned}\hat{f}_{\mathfrak{z}}(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3 r f_{\mathfrak{z}}(\boldsymbol{r}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \\ &= \prod_{\hat{\boldsymbol{\xi}}} (-\mathrm{i})^{\mathfrak{z}\cdot\hat{\boldsymbol{\xi}}} \left[\sqrt{\frac{\pi}{2\alpha}} 2^{\mathfrak{z}\cdot\hat{\boldsymbol{\xi}}} (\mathfrak{z}\cdot\hat{\boldsymbol{\xi}})!\right]^{-1/2} \exp[-\alpha(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}})^2] H_{\mathfrak{z}\cdot\hat{\boldsymbol{\xi}}}(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}}\sqrt{2\alpha}).\end{aligned} \quad (4.15)$$

The proposed decomposition (4.13) has the great merit of showing that the exchange contribution to the energy of the ground state and the low lying excited states of the low density electron system can be neglected in a first approximation. That can be concluded directly from the following two considerations. First of all the coefficients $A^{\sigma_1\ldots\sigma_{2N}}_{\mathfrak{z}_1\ldots\mathfrak{z}_{2N}}(n)$ tend rapidly to zero with increasing $|\mathfrak{z}_1|,\ldots,|\mathfrak{z}_{2N}|$ for the ground state and the low lying excited states. Secondly the overlap between one-electron functions, that are centred around different lattice positions is quite small for small $|\mathfrak{z}_i|$. This follows immediately from the expression for the overlap

$$\begin{aligned}S_{\mathfrak{z}_1\mathfrak{z}_2}(\boldsymbol{R}_{12}) &= \int \mathrm{d}^3 r f^*_{\mathfrak{z}_1}(\boldsymbol{r}-\boldsymbol{R}_1) f_{\mathfrak{z}_2}(\boldsymbol{r}-\boldsymbol{R}_2) \\ &= \exp\left[\frac{-R_{12}^2}{8\alpha}\right] \prod_{\hat{\boldsymbol{\xi}}} \left[\frac{2^{\mathfrak{z}_>\cdot\hat{\boldsymbol{\xi}}} (\mathfrak{z}_<\cdot\hat{\boldsymbol{\xi}})!}{2^{\mathfrak{z}_<\cdot\hat{\boldsymbol{\xi}}} (\mathfrak{z}_>\cdot\hat{\boldsymbol{\xi}})!}\right]^{1/2} \left(\frac{\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}}}{2\sqrt{2\alpha}}\right)^{(\mathfrak{z}_>-\mathfrak{z}_<)\cdot\hat{\boldsymbol{\xi}}} \\ &\quad \times L^{(\mathfrak{z}_>-\mathfrak{z}_<)\cdot\hat{\boldsymbol{\xi}}}_{\mathfrak{z}_<\cdot\hat{\boldsymbol{\xi}}}\left(\frac{(\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right)\end{aligned} \quad (4.16)$$

where $L^{(\mathfrak{z}_>-\mathfrak{z}_<)\cdot\hat{\boldsymbol{\xi}}}_{\mathfrak{z}_<\cdot\hat{\boldsymbol{\xi}}}$ denotes a Laguerre polynomial with $\mathfrak{z}_>\cdot\hat{\boldsymbol{\xi}}$ and $\mathfrak{z}_<\cdot\hat{\boldsymbol{\xi}}$ being the larger and the smaller of the two numbers $\{\mathfrak{z}_1\cdot\hat{\boldsymbol{\xi}}, \mathfrak{z}_2\cdot\hat{\boldsymbol{\xi}}\}$, respectively. Clearly $S_{\mathfrak{z}_1\mathfrak{z}_2}(\boldsymbol{R}_{12})$ is very small at low densities, provided that both the width $\alpha^{1/2}$ of the one-electron functions is small compared with the nearest neighbour distance and the exponential factor dominates (4.16), i.e. $|\mathfrak{z}_1|$ and $|\mathfrak{z}_2|$ should not become too large.

In the following we pay attention to the properties of the low density electron system at low temperatures, i.e. we are only interested in the ground state and the low-lying excited states. Our conclusion that the influence of the exchange energy

on the low temperature properties can be neglected in a first approximation can be expressed mathematically by putting

$$\{d^{+}_{j_1\sigma_1}(R_1), d_{j_2\sigma_2}(R_2)\} = S_{j_1j_2}(R_{12})\delta_{\sigma_1\sigma_2} = \delta_{j_1j_2}\delta_{R_1R_2}\delta_{\sigma_1\sigma_2}. \tag{4.17}$$

The crucial step in our approach is to use the decomposition (4.13) in order to find an effective Hamiltonian with the property

$$H_{\text{eff}}|\psi_n\rangle = E_n|\psi_n\rangle \tag{4.18}$$

where E_n is the approximate energy of the low lying eigenstate $|\psi_n\rangle$ as given in (4.13), i.e. the exchange contribution to the energy spectrum is neglected. The reason for the formulation of an effective Hamiltonian is to analyze the dynamics of the system without taking into account the effect of exchange. In order to construct H_{eff} we first rewrite H, as given in (3.1), in terms of the fermion operators (4.14). For that purpose we use the following relation between plane wavefunctions and oscillator eigenfunctions:

$$\exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}] = (2\pi)^{3/2}\sum_{j} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}} f_j^{*}(\boldsymbol{r}-\boldsymbol{a})\hat{f}_j(\boldsymbol{k}) \tag{4.19}$$

where $\boldsymbol{a}$ denotes the position around which the function f_j is localized. This relation follows directly from the completeness of the set of harmonic oscillator eigenfunctions, i.e.

$$\sum_{j} f_j^{*}(\boldsymbol{r}) f_j(\boldsymbol{r}') = \delta^3(\boldsymbol{r}-\boldsymbol{r}'). \tag{4.20}$$

The required relation between the different sets of fermion operators then reads

$$c^{+}_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{\Omega}}\int \mathrm{d}^3r\,\psi^{+}_{\sigma}(\boldsymbol{r})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2}\sum_{j}\hat{f}_j(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}} d^{+}_{j\sigma}(\boldsymbol{a}). \tag{4.21}$$

Note: the vector $\boldsymbol{a}$ can be arbitrarily chosen. This freedom is essential for obtaining the effective Hamiltonian.

Substitution of (4.21) into (3.1) while taking into account the arbitrariness of $\boldsymbol{a}$ gives rise to the following possible representation of H:

$$H = \sum_{j_1j_2,\sigma} T^{a_1a_2}_{j_1j_2} d^{+}_{j_1\sigma}(\boldsymbol{a}_1) d_{j_2\sigma}(\boldsymbol{a}_2) + \tfrac{1}{2}\sum_{\substack{j_3j_4j_5j_6\\ \sigma,\sigma'}} V^{a_3a_4a_5a_6}_{j_3j_4j_5j_6} d^{+}_{j_3\sigma}(\boldsymbol{a}_3) d^{+}_{j_4\sigma'}(\boldsymbol{a}_4) d_{j_5\sigma'}(\boldsymbol{a}_5) d_{j_6\sigma}(\boldsymbol{a}_6) \tag{4.22}$$

with

$$T^{a_1a_2}_{j_1j_2} = \int \mathrm{d}^3k \frac{\hbar^2k^2}{2m}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{a}_1-\boldsymbol{a}_2)}\hat{f}^{*}_{j_2}(\boldsymbol{k})\hat{f}_{j_1}(\boldsymbol{k}) \tag{4.23}$$

$$V^{a_3a_4a_5a_6}_{j_3j_4j_5j_6} = {\sum_{\boldsymbol{q}}}' \frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{a}_6-\boldsymbol{a}_5)}\left[\int \mathrm{d}^3k\mathrm{d}^3k'\,\hat{f}_{j_3}(\boldsymbol{k})\hat{f}_{j_4}(\boldsymbol{k}')\hat{f}^{*}_{j_5}(\boldsymbol{k}'+\boldsymbol{q})\hat{f}^{*}_{j_6}(\boldsymbol{k}-\boldsymbol{q}) \times \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{a}_3-\boldsymbol{a}_6)}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{a}_4-\boldsymbol{a}_5)}\right]. \tag{4.24}$$

Clearly different sets of vectors a_ℓ, $\ell = 1, 2, \ldots, 6$, correspond with different representations of the same Hamiltonian H, i.e. the eigenfunctions and eigenvalues of H do not depend on the choice of a_ℓ or, to put it differently, the translational symmetry of H is not broken. The reason for introducing the representation (4.22) becomes clear when considering $H|\psi_n\rangle$. Using the decomposition (4.13) and the procedure as given in appendix 1 (cf A1.4) we get

$$\begin{aligned} H|\psi_n\rangle = \sum_{\substack{j_1,\ldots,j_{2N}\\ \sigma_1,\ldots,\sigma_{2N}}} A^{\sigma_1,\ldots,\sigma_{2N}}_{j_1,\ldots,j_{2N}}(n)\Bigg\{ \sum_{i=1}^{2N}(-1)^{2N-i}\Bigg[\prod_{m\neq i} d^+_{j_m\sigma_m}(\boldsymbol{R}_m)\Bigg][H, d^+_{j_i\sigma_i}(\boldsymbol{R}_i)]|\rangle \\ + \sum_{i=1}^{2N}\sum_{j=i+1}^{2N}(-1)^{-i+j+1}\Bigg[\prod_{m\neq i,j} d^+_{j_m\sigma_m}(\boldsymbol{R}_m)\Bigg] \\ \times \{[H, d^+_{j_i\sigma_i}(\boldsymbol{R}_i)], d^+_{j_j\sigma_j}(\boldsymbol{R}_j)\}|\rangle\Bigg\}. \end{aligned} \tag{4.25}$$

The appearing commutators are calculated by using suitably chosen representations of H, i.e. we choose a different set a_ℓ, $\ell = 1, 2, \ldots, 6$, for each commutator. Calling this set $a_1^i, a_2^i, a_3^i, a_4^j, a_5^j, a_6^i$, we arrive at

$$\begin{aligned} [H, d^+_{j_i\sigma_i}(\boldsymbol{R}_i)]|\rangle &= \sum_{s_1 s_2} T^{a_1^i a_2^i}_{s_1 s_2} S_{j_i s_2}(\boldsymbol{R}_i - \boldsymbol{a}_2^i) d^+_{s_1\sigma_i}(\boldsymbol{a}_1^i)|\rangle \\ \{[H, d^+_{j_i\sigma_i}(\boldsymbol{R}_i)], d^+_{j_j\sigma_j}(\boldsymbol{R}_j)\}|\rangle &= \sum_{s_3 s_4 s_5 s_6} V^{a_3^i a_4^j a_5^j a_6^i}_{s_3 s_4 s_5 s_6} \\ &\quad \times S_{j_i s_6}(\boldsymbol{R}_i - \boldsymbol{a}_6^i) S_{j_j s_5}(\boldsymbol{R}_j - \boldsymbol{a}_5^j) d^+_{s_3\sigma_i}(\boldsymbol{a}_3^i) d^+_{s_4\sigma_j}(\boldsymbol{a}_4^j)|\rangle. \end{aligned} \tag{4.26}$$

A further simplification of (4.26) is obtained by the special choice $a_1^i = a_2^i = a_3^i = a_6^i = \boldsymbol{R}_i$ and $a_4^j = a_5^j = \boldsymbol{R}_j$. Then the overlap integrals in (4.26) are equal to one. Now the effective Hamiltonian can be formulated. For the resulting exact expression for $H|\psi_n\rangle$, given by (4.25) and (4.26), can also be obtained by replacing H by the following effective Hamiltonian H_{eff}, provided that the overlap terms are neglected:

$$\begin{aligned} H_{\text{eff}} = \sum_{i, j_1, j_2, \sigma} T_{j_1 j_2} d^+_{j_1\sigma}(\boldsymbol{R}_i) d_{j_2\sigma}(\boldsymbol{R}_i) \\ + \tfrac{1}{2}\sum_{i\neq j}\sum_{j_3 j_4 j_5 j_6, \sigma\sigma'} V^{ij}_{j_3 j_4 j_5 j_6} d^+_{j_3\sigma}(\boldsymbol{R}_i) d^+_{j_4\sigma'}(\boldsymbol{R}_j) d_{j_5\sigma'}(\boldsymbol{R}_j) d_{j_6\sigma}(\boldsymbol{R}_i) \end{aligned} \tag{4.27}$$

where

$$\begin{aligned} T_{j_1 j_2} &= \int \mathrm{d}^3 k \frac{\hbar^2 k^2}{2m} \hat{f}_{j_2}(\boldsymbol{k}) \hat{f}_{j_1}(\boldsymbol{k}) \\ &= \sum_{\hat{\xi}\in\{\hat{x},\hat{y},\hat{z}\}} \frac{\hbar^2}{4m\alpha}\Big[\delta_{j_1 j_2}(j_1\cdot\hat{\xi} + \tfrac{1}{2}) - \tfrac{1}{2}\delta_{j_1, j_2+2\hat{\xi}}\sqrt{(j_2\cdot\hat{\xi}+1)(j_2\cdot\hat{\xi}+2)} \\ &\quad - \tfrac{1}{2}\delta_{j_2, j_1+2\hat{\xi}}\sqrt{(j_1\cdot\hat{\xi}+1)(j_1\cdot\hat{\xi}+2)}\Big] \end{aligned} \tag{4.28}$$

and

$$V^{ij}_{j_3j_4j_5j_6} = \sum_q{}' \frac{4\pi e^2}{\Omega q^2} e^{iq\cdot R_{ij}} \int d^3k d^3k' \hat{f}_{j_3}(k)\hat{f}_{j_4}(k')\hat{f}^*_{j_5}(k'+q)\hat{f}^*_{j_6}(k-q) \tag{4.29}$$

with

$$\int d^3k \hat{f}_{\ell_1}(k)\hat{f}^*_{\ell_2}(k\pm q) = e^{-\frac{1}{2}\alpha q^2}\prod_{\hat{\xi}}\left[\frac{2^{\ell_>\cdot\hat{\xi}}(\ell_<\cdot\hat{\xi})}{2^{\ell_<\cdot\hat{\xi}}(\ell_>\cdot\hat{\xi})}\right]^{1/2}(\pm i\tfrac{1}{2}\sqrt{2\alpha}q\cdot\hat{\xi})^{(\ell_>-\ell_<)\cdot\hat{\ell}} L^{(\ell_>-\ell_<)\cdot\hat{\xi}}_{\ell_<\cdot\hat{\xi}}(\alpha(q\cdot\hat{\xi})^2). \tag{4.30}$$

The Hamiltonian (4.27) does not take into account the effect of exchange on the dynamics of the electrons. Note that the original translation symmetry is broken in H_{eff}.

Next H_{eff} is expressed in terms of the following electron-hole operators.

$$D^i_{j_1j_2} = \sum_\sigma d^+_{j_1\sigma}(R_i)d_{j_2\sigma}(R_i). \tag{4.31}$$

Substituting (4.31) into (4.27) we obtain

$$H_{\text{eff}} = \sum_i\sum_{j_1j_2} T_{j_1j_2}D^i_{j_1j_2} + \tfrac{1}{2}\sum_{i\neq j}\sum_{j_3j_4j_5j_6} V^{ij}_{j_3j_4j_5j_6}D^i_{j_3j_6}D^j_{j_4j_5}. \tag{4.32}$$

The operators $D^i_{j_1j_2}$ satisfy the commutation relations

$$[D^i_{j_1j_2}, D^j_{j_3j_4}] = \delta_{ij}[\delta_{j_2j_3}D^i_{j_1j_4} - \delta_{j_1j_4}D^i_{j_3j_2}]. \tag{4.33}$$

Considering only the low lying eigenstates $|\psi_n\rangle$ and neglecting the overlap we can also use the following effective properties

$$\sum_j D^i_{jj} = 1 \tag{4.34}$$

and

$$D^i_{j_1j_2}D^i_{j_3j_4} = \delta_{j_2j_3}D^i_{j_1j_4}. \tag{4.35}$$

Wigner's result follows directly by choosing the ground state $|\psi_0\rangle$ equal to $|\Psi_{\text{HF}}\rangle$ as given in (3.7). Then the ground state energy is approximated by

$$E_0 = \langle\Psi_{\text{HF}}|H_{\text{eff}}|\Psi_{\text{HF}}\rangle = 2NT_{00} + \tfrac{1}{2}\sum_{i\neq j}V^{ij}_{0000}$$
$$= 2N\frac{3\hbar^2}{8m\alpha} + \tfrac{1}{2}\sum_{i\neq j}\sum_q{}'\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}\exp[iq\cdot R_{ij}]. \tag{4.36}$$

Minimizing E_0 with respect to α and neglecting all terms containing $\operatorname{erfc}(R_{ij}/2\sqrt{\alpha})$ leads to Wigner's ground state energy.

In order to take into account the electron–electron correlation we substitute first

$$L^{(\ell_>-\ell_<)\cdot\hat{\xi}}_{\ell_<\cdot\hat{\xi}}(\alpha(q\cdot\hat{\xi})^2)=\sum_{m=0}^{\ell_<\cdot\hat{\xi}}(-1)^m\binom{\ell_>\cdot\hat{\xi}}{\ell_<\cdot\hat{\xi}-m}\frac{[\alpha(q\cdot\hat{\xi})^2]^m}{m!} \tag{4.37}$$

into the matrix elements $V^{ij}_{\jmath_3\jmath_4\jmath_5\jmath_6}$. As shown in appendix 5 that leads to the following expression for the interaction operator V of an electron lattice with cubic symmetry:

$$\begin{aligned}V=E_{\mathrm{Cl}}+\tfrac{1}{2}\sum_{i\neq j}\sum_{q}{}'\,\mathrm{e}^{\mathrm{i}q\cdot R_{ij}}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}\{\tfrac{1}{2}\alpha[\mathrm{i}q\cdot(S_i-S_j)]^2\\ +\tfrac{1}{6}\alpha\sqrt{\alpha}[\mathrm{i}q\cdot(S_i-S_j)]^3+\tfrac{1}{24}\alpha^2[\mathrm{i}q\cdot(S_i-S_j)]^4\}\end{aligned} \tag{4.38}$$

where terms containing q^n, $n>4$, are neglected and the operators S_i are given by

$$S_i=\sum_{\hat{\xi}}\hat{\xi}S^i_{\hat{\xi}} \tag{4.39}$$

with

$$S^i_{\hat{\xi}}=\sum_{\jmath}\sqrt{\jmath\cdot\hat{\xi}+1}\,[D^i_{\jmath+\hat{\xi},\jmath}+D^i_{\jmath,\jmath+\hat{\xi}}]. \tag{4.40}$$

Now H_{eff} can be treated exactly up to order $(S_i-S_j)^2$. In that case the relevant interaction operator reads

$$V=E_{\mathrm{Cl}}+\tfrac{1}{2}\sum_{i\neq j}\sum_{q}{}'\,\mathrm{e}^{\mathrm{i}q\cdot R_{ij}}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}\sum_{\hat{\xi},\hat{\eta}}\alpha(q\cdot\hat{\xi})(q\cdot\hat{\eta})[S^i_{\hat{\xi}}S^j_{\hat{\eta}}-\tfrac{1}{2}S^i_{\hat{\xi}}S^i_{\hat{\eta}}-\tfrac{1}{2}S^j_{\hat{\xi}}S^j_{\hat{\eta}}] \tag{4.41}$$

with

$$\begin{aligned}\sum_{q}{}'\,\mathrm{e}^{\mathrm{i}q\cdot R_{ij}}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}(q\cdot\hat{\xi})(q\cdot\hat{\eta})\\ =-e^2\Big[\delta_{\hat{\xi}\hat{\eta}}\Big(\frac{\exp(-R^2_{ij}/4\alpha)}{\sqrt{\pi\alpha}R^2_{ij}}+\frac{\operatorname{erfc}(R_{ij}/2\sqrt{\alpha})}{R^3_{ij}}-\frac{1}{R^3_{ij}}\Big)\\ +(R_{ij}\cdot\hat{\xi})(R_{ij}\cdot\hat{\eta})\Big[\frac{3}{R^5_{ij}}-\frac{3\operatorname{erfc}(R_{ij}/2\sqrt{\alpha})}{R^5_{ij}}-\frac{\exp(-R^2_{ij}/4\alpha)}{R^2_{ij}}\\ \times\Big(\frac{1}{2\alpha\sqrt{\pi\alpha}}+\frac{3}{R^2_{ij}\sqrt{\pi\alpha}}\Big)\Big]\Big]\end{aligned} \tag{4.42}$$

and

$$\begin{aligned}\tfrac{1}{2}\sum_{R_i\neq 0}\sum_{q}{}'\,\mathrm{e}^{\mathrm{i}q\cdot R_i}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}(q\cdot\hat{\xi})(q\cdot\hat{\eta})\\ =\delta_{\hat{\xi}\hat{\eta}}\Big[\frac{-4\pi Ne^2}{3\Omega}+\sum_{R_i\neq 0}\mathrm{e}^{-R_i^2/4\alpha}\frac{e^2}{12\alpha\sqrt{\pi\alpha}}\Big]\end{aligned} \tag{4.43}$$

where use is made of the cubic symmetry of the lattice in the last calculation. Neglecting the terms in (4.42) and (4.43) of the order of the overlap, i.e. terms containing $\exp(-R_{ij}^2/4\alpha)$ and $\operatorname{erfc}(R_{ij}/2\sqrt{\alpha})$, we arrive at

$$V = E_{\mathrm{Cl}} + \tfrac{1}{2}\alpha \sum_{i,j} \sum_{\hat{\xi},\hat{\eta}} M_{\hat{\xi}\hat{\eta}}(\boldsymbol{R}_{ij}) S_{\hat{\xi}}^i S_{\hat{\eta}}^j \tag{4.44}$$

where the elements of the second rank tensor $M(\boldsymbol{R}_{ij})$ are given by

$$\begin{aligned} M_{\hat{\xi}\hat{\eta}}(\boldsymbol{R}_{ij}) &= e^2\left[\frac{1}{R_{ij}^3}\delta_{\hat{\xi}\hat{\eta}} - \frac{3}{R_{ij}^5}(\boldsymbol{R}_{ij}\cdot\hat{\xi})(\boldsymbol{R}_{ij}\cdot\hat{\eta})\right] \qquad \text{for } i \neq j \\ M_{\hat{\xi}\hat{\eta}}(0) &= \frac{8\pi N e^2}{3\Omega}\delta_{\hat{\xi}\hat{\eta}}. \end{aligned} \tag{4.45}$$

These tensor elements are identical to the elements $M(\boldsymbol{R}_{ij})_{\mu\nu}$, with $\mu,\nu = x,y,z$, as given by (4.2).

The kinetic energy term T reads according to (4.28) and (4.32):

$$T = \frac{\hbar^2}{4m\alpha} \sum_i \sum_{\hat{\xi}} \sum_{\jmath} \left[(\tfrac{1}{2} + \jmath\cdot\hat{\xi}) D_{\jmath\jmath}^i - \tfrac{1}{2}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)}\,(D_{\jmath,\jmath+2\hat{\xi}}^i + D_{\jmath+2\hat{\xi},\jmath}^i)\right]. \tag{4.46}$$

Introducing the operators

$$P_{\hat{\xi}}^i = \sum_{\jmath} \sqrt{\jmath\cdot\hat{\xi}+1}\,[D_{\jmath,\jmath+\hat{\xi}}^i - D_{\jmath+\hat{\xi},\jmath}^i] \tag{4.47}$$

we obtain using (4.35):

$$T = -\frac{\hbar^2}{8m\alpha} \sum_{i,\hat{\xi}} P_{\hat{\xi}}^i P_{\hat{\xi}}^i. \tag{4.48}$$

Thus H_{eff} can be expressed as the following bilinear form:

$$H_{\mathrm{eff}} = -\frac{\hbar^2}{8m\alpha} \sum_{i,\hat{\xi}} P_{\hat{\xi}}^i P_{\hat{\xi}}^i + E_{\mathrm{Cl}} + \tfrac{1}{2}\alpha \sum_{i,j} \sum_{\hat{\xi},\hat{\eta}} M_{\hat{\xi}\hat{\eta}}(\boldsymbol{R}_{ij}) S_{\hat{\xi}}^i S_{\hat{\eta}}^j. \tag{4.49}$$

In order to determine the eigenvalues of H_{eff} we make use of the commutator

$$[P_{\hat{\xi}}^i, S_{\hat{\eta}}^j] = \delta_{ij}\delta_{\hat{\xi}\hat{\eta}} \sum_{\jmath} 2 D_{\jmath\jmath}^i = 2\delta_{ij}\delta_{\hat{\xi}\hat{\eta}} \tag{4.50}$$

which holds because of (4.33) and (4.34). Then H_{eff} can be diagonalized analogous to Carr's procedure. Introducing

$$\begin{aligned} S_{k\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\xi}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{e}_{-k\lambda}\cdot\hat{\xi} S_{\hat{\xi}}^i \\ P_{k\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\xi}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{e}_{k\lambda}\cdot\hat{\xi} P_{\hat{\xi}}^i \end{aligned} \tag{4.51}$$

we arrive at

$$H_{\text{eff}} = E_{\text{CI}} - \frac{\hbar^2}{8m\alpha}\sum_{k\lambda} P_{k\lambda}P_{-k\lambda} + \tfrac{1}{2}\alpha\sum_{k\lambda} m\omega_{k\lambda}^2 S_{-k\lambda}S_{k\lambda} \tag{4.52}$$

where $\varepsilon_{k\lambda}$ and $\omega_{k\lambda}$ are given by the eigenvalue equation (4.4). The operators $S_{k\lambda}$ and $P_{k\lambda}$ satisfy

$$\begin{aligned}&[S_{k\lambda}, S_{k'\lambda'}] = [P_{k\lambda}, P_{k'\lambda'}] = 0\\ &[P_{k\lambda}, S_{k'\lambda'}] = \frac{1}{2N}\sum_{i,j} 2D_{ij}^{i}\mathrm{e}^{\mathrm{i}(k-k')R_i}\varepsilon_{k\lambda}\cdot\varepsilon_{-k'\lambda'} = 2\delta_{kk'}\delta_{\lambda\lambda'}.\end{aligned} \tag{4.53}$$

The effective Hamiltonian (4.52) can be rewritten in terms of the boson operators

$$\begin{aligned}A_{k\lambda} &= \sqrt{\frac{m\omega_{k\lambda}\alpha}{2\hbar}}S_{k\lambda} + \sqrt{\frac{\hbar}{8m\omega_{k\lambda}\alpha}}P_{-k\lambda}\\ A_{k\lambda}^{+} &= \sqrt{\frac{m\omega_{k\lambda}\alpha}{2\hbar}}S_{-k\lambda} - \sqrt{\frac{\hbar}{8m\omega_{k\lambda}\alpha}}P_{k\lambda}\end{aligned} \tag{4.54}$$

that satisfy the commutation relations

$$\begin{aligned}&[A_{k\lambda}, A_{k'\lambda'}] = [A_{k\lambda}^{+}, A_{k'\lambda'}^{+}] = 0\\ &[A_{k\lambda}, A_{k'\lambda'}^{+}] = \delta_{kk'}\delta_{\lambda\lambda'}.\end{aligned} \tag{4.55}$$

Then the effective Hamiltonian is

$$H_{\text{eff}} = E_{\text{CI}} + \sum_{k\lambda}\hbar\omega_{k\lambda}[\tfrac{1}{2} + A_{k\lambda}^{+}A_{k\lambda}]. \tag{4.56}$$

The corresponding internal energy is given by

$$E = E_{\text{CI}} + \sum_{k\lambda}\left[\frac{1}{2} + \frac{1}{\exp(\beta\hbar\omega_{k\lambda}) - 1}\right]\hbar\omega_{k\lambda} \tag{4.57}$$

where $\beta = 1/k_{\text{B}}T$ with k_{B} and T denoting the Boltzmann constant and temperature, respectively.

As to the internal energy (4.57) the following remarks should be made. First of all it only holds provided that exchange terms can be neglected. Such an approximation is only valid for the low density electron system at low temperatures. For the statistical weight of the higher excited states $|\psi_n\rangle$ increases with temperature, meaning that even at low density the overlap is not negligible at higher temperatures. The ground state energy is exact up to order $r_s^{-3/2}$. The terms of order $(\boldsymbol{S}_i - \boldsymbol{S}_j)^n$, $n > 2$, which were also neglected, can be dealt with as a perturbation and give rise to terms of the order of $r_s^{-2}, r_s^{-5/2}, r_s^{-3}, \ldots$ in the ground state energy (see appendix 5).

Carr's approach and ours become mathematically identical when identifying $\boldsymbol{r}_i - \boldsymbol{R}_i$ with $\sqrt{\alpha}\boldsymbol{S}_i$ and $a_{k\lambda}^{(+)}$ with $A_{k\lambda}^{(+)}$. That identity does not only hold for Carr's harmonic term and our $(\boldsymbol{S}_i - \boldsymbol{S}_j)^2$ term but also for his anharmonic terms

and our corresponding $(S_i - S_j)^n$ terms. Consequently the energy terms of order r_s^{-2}, $r_s^{-5/2}$, r_s^{-3}, ... can be calculated according to the theory of anharmonic lattices [11–13].

Finally we discuss the already mentioned epistomological questions arising from the semiclassical nature of Carr's approach.

(i) Carr's results can be obtained indeed in a fully quantum mechanical way. Although the terms of our effective Hamiltonian and the corresponding ones of Carr's expansion can be treated in a mathematically identical way, the present approach does not break the permutation symmetry. Therefore our effective Hamiltonian cannot result from Carr's expansion.

(ii) The low density electron system can indeed be effectively described up to order $r_s^{-3/2}$ in terms of a system of free bosons, provided that exchange is neglected. The appearing boson operators $A_{k\lambda}^{(+)}$ are bilinear expressions of the original fermion operators as follows from (4.31), (4.40), (4.47), (4.51) and (4.54).

(iii) The ground state $|\psi_0\rangle$ of the effective Hamiltonian (4.56) is obtained by requiring

$$A_{k\lambda}|\psi_0\rangle = 0 \tag{4.58}$$

for all k and λ. As shown in appendix 6 the requirement (4.58) gives rise to relations between the coefficients $A_{j_1,\ldots,j_{2N}}^{\sigma_1,\ldots,\sigma_{2N}}(0)$ of the decomposition (4.13) that completely determine $|\psi_0\rangle$. It should be remarked here that the correlated ground state $|\psi_0\rangle$ still depends on a seemingly free parameter α. However, although the energy (4.57) does not depend on α, the choice of α is restricted by the requirement that overlap must be negligible for large r_s. This means that the width $\alpha^{1/2}$ of the harmonic oscillator wavefunctions must be small compared with the nearest neighbour distance.

5. The effect of a magnetic field on the Wigner lattice

A detailed study of the properties of the three-dimensional low-density electron system in the presence of a magnetic field has never been published, as far as we know. The results as obtained by Fukuyama [14,15] and Fukuyama and McClure [16] in their study of the two-dimensional case with the field perpendicular to the lattice plane cannot be simply generalized to three dimensions. For the macroscopic magnetic field is no longer the applied external field but an internal field, that must be determined self-consistently. This is done as follows. First an *ansatz* is chosen for the magnetic field. Next the response of the system to that field is calculated. Then the internal field is calculated by means of Maxwell's equations with the response as source term and compared with the *ansatz*. In case of difference the procedure is repeated starting from the calculated field, until self-consistency is obtained.

In subsection 5.1 we use the described procedure to show that the low-density jellium model allows a homogeneous internal field. Besides the effect of this field on the ground state energy of the Wigner lattice is calculated exactly up to order $r_s^{-3/2}$. The strength of the internal field cannot be calculated as boundary conditions are absent here. This means that it is unclear whether a field can actually penetrate into the system. For that reason in subsection 5.2 we pay attention to the effect of boundary conditions by considering the response to an inhomogeneous field. It appears that the system does not show the Meissner–Ochsenfeld effect, i.e. the field does penetrate the system.

5.1. Homogeneous magnetic field

In order to show that the jellium model allows a homogeneous magnetic field we take a constant internal field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ as an *ansatz*. The jellium model in the presence of such a field is described in terms of the Hamiltonian

$$H = \sum_{\sigma} \int \mathrm{d}^3 r \psi_\sigma^+(\boldsymbol{r}) \left[\frac{\hbar}{\mathrm{i}}\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right]^2 \frac{1}{2m} \psi_\sigma(\boldsymbol{r}) + \tfrac{1}{2}{\sum_{\boldsymbol{q}}}' \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\sigma,\sigma'} V(\boldsymbol{q}) c_{\boldsymbol{k}\sigma}^+ c_{\boldsymbol{k}'\sigma'}^+ c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} - \mu_{\mathrm{B}} B \sum_{\boldsymbol{k}} [c_{\boldsymbol{k}\uparrow}^+ c_{\boldsymbol{k}\uparrow} - c_{\boldsymbol{k}\downarrow}^+ c_{\boldsymbol{k}\downarrow}] \tag{5.1}$$

where $\boldsymbol{A}$ is the vector potential defined by $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ and μ_{B} is the Bohr magneton $e\hbar/2mc$. The last term in (5.1) describes the interaction of the electron spins with the magnetic field. The vector potential is chosen according to the symmetric gauge:

$$\boldsymbol{A}(\boldsymbol{r}) = \tfrac{1}{2}\boldsymbol{B} \times \boldsymbol{r} = \tfrac{1}{2}B[x\hat{\boldsymbol{y}} - y\hat{\boldsymbol{x}}]. \tag{5.2}$$

In order to calculate the energy spectrum and the low-lying eigenstates of the Hamiltonian (5.1) up to order $r_s^{-3/2}$ the procedure of section 4 is followed. The underlying assumption is that a small magnetic field does not destroy the Wigner lattice, i.e. the effect of exchange on the energies of the low-lying eigenstates is negligible for low densities. The behaviour of the quantum mechanical Wigner lattice is analogous to that of the classical lattice. Thus we can choose the positions of the lattice to be time-independent. It should be noted that the situation is quite different for an electric field. For each site $\boldsymbol{R}_i$, $i = 1, \ldots, 2N$, a complete set of one-electron functions that depend on the magnetic field B and the lattice site $\boldsymbol{R}_i$ is chosen. These functions $f_{\jmath\boldsymbol{R}_i}^B$ are localized at $\boldsymbol{R}_i$ in such a way that their mutual overlap can be neglected for small $|\jmath|$.

The eigenstates of (5.1) can be written as (cf (4.13))

$$|\psi_n^B\rangle = \sum_{\substack{\jmath_1,\ldots,\jmath_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} A_{\jmath_1\ldots\jmath_{2N}}^{\sigma_1\ldots\sigma_{2N}}(B,n) d_{B\jmath_1\sigma_1}^+(\boldsymbol{R}_1)\ldots d_{B\jmath_{2N}\sigma_{2N}}^+(\boldsymbol{R}_{2N})|\rangle \tag{5.3}$$

where the fermion operators $d_{B\jmath_i\sigma_i}^+(\boldsymbol{R}_i)$ are defined as

$$d_{B\jmath_i\sigma_i}^+(\boldsymbol{R}_i) = \int \mathrm{d}^3 r \psi_{\sigma_i}^+(\boldsymbol{r}) f_{\jmath_i\boldsymbol{R}_i}^B(\boldsymbol{r} - \boldsymbol{R}_i) = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i] \hat{f}_{\jmath_i\boldsymbol{R}_i}^B(\boldsymbol{k}) c_{\boldsymbol{k}\sigma_i}^+ \tag{5.4}$$

with $\hat{f}_{\jmath_i\boldsymbol{R}_i}^B$ being the Fourier transform of $f_{\jmath_i\boldsymbol{R}_i}^B$.

Because the effect of exchange is neglected for low densities and low temperatures in a first approximation we can replace the original Hamiltonian (5.1) by the following effective Hamiltonian:

$$H_{\mathrm{eff}} = \sum_{i} \sum_{\jmath_1\jmath_2\sigma} T_{B\jmath_1\jmath_2}^i d_{B\jmath_1\sigma}^+(\boldsymbol{R}_i) d_{B\jmath_2\sigma}(\boldsymbol{R}_i)$$

$$+\tfrac{1}{2}\sum_{i\neq j}\sum_{\substack{\jmath_3\jmath_4\jmath_5\jmath_6\\ \sigma,\sigma'}} V^{ij}_{B_{\jmath_3}B_{\jmath_4}B_{\jmath_5}B_{\jmath_6}} d^{+}_{B_{\jmath_3}\sigma}(\boldsymbol{R}_i)d^{+}_{B_{\jmath_4}\sigma'}(\boldsymbol{R}_j)d_{B_{\jmath_5}\sigma'}(\boldsymbol{R}_j)d_{B_{\jmath_6}\sigma}(\boldsymbol{R}_i)$$

$$-\mu_B B\sum_i\sum_{\jmath_7\jmath_8} U^{i}_{B_{\jmath_7}B_{\jmath_8}}[d^{+}_{B_{\jmath_7}\uparrow}(\boldsymbol{R}_i)d_{B_{\jmath_8}\uparrow}(\boldsymbol{R}_i)-d^{+}_{B_{\jmath_7}\downarrow}(\boldsymbol{R}_i)d_{B_{\jmath_8}\downarrow}(\boldsymbol{R}_i)] \tag{5.5}$$

where

$$T^{i}_{B_{\jmath_1}B_{\jmath_2}}=\int \mathrm{d}^3r\, f^{B}_{\jmath_1\boldsymbol{R}_i}(\boldsymbol{r}-\boldsymbol{R}_i)\left[\frac{\hbar}{\mathrm{i}}\nabla-\frac{eB}{2c}(x\hat{\boldsymbol{y}}-y\hat{\boldsymbol{x}})\right]^2\frac{1}{2m}f^{*B}_{\jmath_2\boldsymbol{R}_i}(\boldsymbol{r}-\boldsymbol{R}_i) \tag{5.6}$$

$$V^{ij}_{B_{\jmath_3}B_{\jmath_4}B_{\jmath_5}B_{\jmath_6}}=\sum_{\boldsymbol{q}}{}'\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_{ij}}\int \mathrm{d}^3k\mathrm{d}^3k'\,\hat{f}^{B}_{\jmath_3\boldsymbol{R}_i}(\boldsymbol{k})\hat{f}^{B}_{\jmath_4\boldsymbol{R}_j}(\boldsymbol{k}')\hat{f}^{*B}_{\jmath_5\boldsymbol{R}_j}(\boldsymbol{k}'+\boldsymbol{q})\hat{f}^{*B}_{\jmath_6\boldsymbol{R}_i}(\boldsymbol{k}-\boldsymbol{q}) \tag{5.7}$$

and

$$U^{i}_{B_{\jmath_7}B_{\jmath_8}}=\int \mathrm{d}^3k\,\hat{f}^{B}_{\jmath_7\boldsymbol{R}_i}(\boldsymbol{k})\hat{f}^{*B}_{\jmath_8\boldsymbol{R}_i}(\boldsymbol{k}). \tag{5.8}$$

Clearly the low-lying states of H_{eff} and their attendant energies do not depend on the choice of the functions $f^{B}_{\jmath\boldsymbol{R}_i}$ as these functions are chosen to satisfy the following requirements:

(i) they must form a complete set for each lattice site $\boldsymbol{R}_i$;
(ii) their mutual overlap must be negligible for small $|\jmath|$.

As will be shown a very convenient choice is

$$f^{B}_{\jmath\boldsymbol{R}_i}(\boldsymbol{r}-\boldsymbol{R}_i)=\exp\left[\mathrm{i}\boldsymbol{R}_i\frac{eB}{2c\hbar}(y\hat{\boldsymbol{x}}-x\hat{\boldsymbol{y}})\right]f_\jmath(\boldsymbol{r}-\boldsymbol{R}_i) \tag{5.9}$$

where $f_\jmath$ is the harmonic oscillator eigenfunction (4.12). Then the Fourier transform is given by

$$\hat{f}^{B}_{\jmath\boldsymbol{R}_i}(\boldsymbol{k})=\hat{f}_\jmath\left(\boldsymbol{k}-\frac{e}{2c\hbar}[\boldsymbol{R}_i\times\boldsymbol{B}]\right) \tag{5.10}$$

with $\hat{f}_\jmath$ being the Fourier transform (4.15) of the function (4.12). The functions (5.9) have the required properties as can easily be checked.

(i) They form a complete set as follows from the completeness of the harmonic oscillator eigenfunctions.

(ii) The overlap between functions localized around different lattice sites $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ is given by (cf (4.16))

$$\begin{aligned}S^{B}_{\jmath_1\jmath_2}(\boldsymbol{R}_{12})&=\int \mathrm{d}^3r\, f^{*B}_{\jmath_1\boldsymbol{R}_1}(\boldsymbol{r}-\boldsymbol{R}_1)f^{B}_{\jmath_2\boldsymbol{R}_2}(\boldsymbol{r}-\boldsymbol{R}_2)\\ &=\exp\left[\frac{-R_{12}^2}{8\alpha}-\tfrac{1}{2}\alpha\left[\boldsymbol{R}_{12}\times\frac{Be}{2c\hbar}\right]^2\right]\prod_{\hat{\boldsymbol{\xi}}}\left[\frac{2^{\jmath_>\cdot\hat{\boldsymbol{\xi}}}(\jmath_<\cdot\hat{\boldsymbol{\xi}})!}{2^{\jmath_<\cdot\hat{\boldsymbol{\xi}}}(\jmath_>\cdot\hat{\boldsymbol{\xi}})!}\right]^{1/2}\\ &\quad\times\left[\left(\frac{\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}}+2\mathrm{i}\alpha[\boldsymbol{R}_{12}\times Be/2c\hbar]\cdot\hat{\boldsymbol{\xi}}}{2\sqrt{2\alpha}}\right)^{(\jmath_>-\jmath_<)\cdot\hat{\boldsymbol{\xi}}}\right.\\ &\quad\left.\times L^{(\jmath_>-\jmath_<)\cdot\hat{\boldsymbol{\xi}}}_{\jmath_<\cdot\hat{\boldsymbol{\xi}}}\left(\frac{(\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}})^2+4\alpha^2([\boldsymbol{R}_{12}\times Be/2c\hbar]\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right)\right]\end{aligned} \tag{5.11}$$

and can indeed be neglected at low densities for small $|\mathfrak{z}_1|$ and $|\mathfrak{z}_2|$.

Now the reason for our choice of the functions $f^B_{\mathfrak{z}R_i}$ is clear. For the matrix elements $T^i_{B\mathfrak{z}_1\mathfrak{z}_2}$ do not depend on R_i due to the phase factor in (5.9). Further the factor does not appear in the matrix elements $V^{ij}_{B\mathfrak{z}_3\mathfrak{z}_4\mathfrak{z}_5\mathfrak{z}_6}$ and $U^i_{B\mathfrak{z}_7\mathfrak{z}_8}$ as well. Substitution of (5.9) and (5.10) into (5.6), (5.7) and (5.8), respectively, gives

$$\begin{aligned}
T_{B\mathfrak{z}_1\mathfrak{z}_2} &= \int \mathrm{d}^3 r f_{\mathfrak{z}_1}(r)\left[\frac{\hbar}{\mathrm{i}}\nabla - \frac{eB}{2c}(x\hat{y} - y\hat{x})\right]^2 \frac{1}{2m} f^*_{\mathfrak{z}_2}(r) \\
&= \sum_{\hat{\xi}\in\{\hat{x},\hat{y},\hat{z}\}} \frac{\hbar^2}{4m\alpha}\Big[\delta_{\mathfrak{z}_1\mathfrak{z}_2}(\mathfrak{z}_1\cdot\hat{\xi}+\tfrac{1}{2}) - \tfrac{1}{2}\delta_{\mathfrak{z}_1,\mathfrak{z}_2+2\hat{\xi}}\sqrt{(\mathfrak{z}_2\cdot\hat{\xi}+1)(\mathfrak{z}_2\cdot\hat{\xi}+2)} \\
&\quad - \tfrac{1}{2}\delta_{\mathfrak{z}_2,\mathfrak{z}_1+2\hat{\xi}}\sqrt{(\mathfrak{z}_1\cdot\hat{\xi}+1)(\mathfrak{z}_1\cdot\hat{\xi}+2)}\Big] \\
&\quad + \mathrm{i}\mu_B B\Big[\delta_{\mathfrak{z}_1+\hat{x},\mathfrak{z}_2+\hat{y}}\sqrt{(\mathfrak{z}_1\cdot\hat{x}+1)(\mathfrak{z}_2\cdot\hat{y}+1)} \\
&\quad - \delta_{\mathfrak{z}_2+\hat{x},\mathfrak{z}_1+\hat{y}}\sqrt{(\mathfrak{z}_1\cdot\hat{y}+1)(\mathfrak{z}_2\cdot\hat{x}+1)}\Big] \\
&\quad + \mu_B^2 B^2 \frac{m\alpha}{\hbar^2}\sum_{\hat{\xi}\in\{\hat{x},\hat{y}\}}\Big[\delta_{\mathfrak{z}_1\mathfrak{z}_2}(\mathfrak{z}_1\cdot\hat{\xi}+\tfrac{1}{2}) \\
&\quad + \tfrac{1}{2}\delta_{\mathfrak{z}_1,\mathfrak{z}_2+2\hat{\xi}}\sqrt{(\mathfrak{z}_2\cdot\hat{\xi}+1)(\mathfrak{z}_2\cdot\hat{\xi}+2)} \\
&\quad + \tfrac{1}{2}\delta_{\mathfrak{z}_2,\mathfrak{z}_1+2\hat{\xi}}\sqrt{(\mathfrak{z}_1\cdot\hat{\xi}+1)(\mathfrak{z}_1\cdot\hat{\xi}+2)}\Big] \qquad (5.12)
\end{aligned}$$

$$V^{ij}_{B\mathfrak{z}_3\mathfrak{z}_4\mathfrak{z}_5\mathfrak{z}_6} = V^{ij}_{\mathfrak{z}_3\mathfrak{z}_4\mathfrak{z}_5\mathfrak{z}_6} \qquad (5.13)$$

$$U^i_{B\mathfrak{z}_7\mathfrak{z}_8} = \int \mathrm{d}^3 k \hat{f}_{\mathfrak{z}_7}(k)\hat{f}^*_{\mathfrak{z}_8}(k) = \delta_{\mathfrak{z}_7\mathfrak{z}_8}. \qquad (5.14)$$

The matrix elements (5.13) are given by (4.29).

In terms of the operators

$$D^i_{B\mathfrak{z}_1\mathfrak{z}_2} = \sum_\sigma d^+_{B\mathfrak{z}_1\sigma}(R_i)d_{B\mathfrak{z}_2\sigma}(R_i) \qquad (5.15)$$

and the operators Σ_{Bi} defined by

$$\Sigma_{Bi} = \sum_{\mathfrak{z}} d^+_{B\mathfrak{z}\uparrow}(R_i)d_{B\mathfrak{z}\downarrow}(R_i) \qquad (5.16)$$

the effective Hamiltonian can be rewritten as

$$\begin{aligned}
H_{\mathrm{eff}} = \sum_{i,\mathfrak{z}}\Big[&\frac{\hbar^2}{4m\alpha}\sum_{\hat{\xi}}\Big[(\mathfrak{z}\cdot\hat{\xi}+\tfrac{1}{2})D^i_{B\mathfrak{z}\mathfrak{z}} \\
&- \tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}(D^i_{B\mathfrak{z},\mathfrak{z}+2\hat{\xi}} + D^i_{B\mathfrak{z}+2\hat{\xi},\mathfrak{z}})\Big] \\
&+ \mathrm{i}\mu_B B\Big[\sqrt{(\mathfrak{z}\cdot\hat{y}+1)(\mathfrak{z}\cdot\hat{x}+1)}(D^i_{B\mathfrak{z}+\hat{y},\mathfrak{z}+\hat{x}} - D^i_{B\mathfrak{z}+\hat{x},\mathfrak{z}+\hat{y}})\Big]
\end{aligned}$$

$$+\mu_B^2 B^2 \frac{m\alpha}{\hbar^2} \sum_{\hat{\xi}\in\{\hat{x},\hat{y}\}} \Big[(\mathfrak{z}\cdot\hat{\xi}+\tfrac{1}{2}) D^i_{B\mathfrak{z}\mathfrak{z}} + \tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}\,(D^i_{B\mathfrak{z},\mathfrak{z}+2\hat{\xi}} - D^i_{B\mathfrak{z}+2\hat{\xi},\mathfrak{z}}) \Big] \Big]$$
$$+\tfrac{1}{2}\sum_{i\neq j}\sum_{\mathfrak{z}_1\mathfrak{z}_4\mathfrak{z}_5\mathfrak{z}_6} V^{ij}_{\mathfrak{z}_1\mathfrak{z}_4\mathfrak{z}_5\mathfrak{z}_6} D^i_{B\mathfrak{z}_1\mathfrak{z}_6} D^j_{B\mathfrak{z}_4\mathfrak{z}_5} - \mu_B B \sum_i [\Sigma_{Bi}\Sigma^+_{Bi} - \Sigma^+_{Bi}\Sigma_{Bi}] \tag{5.17}$$

where use has been made of (5.12), (5.13), (5.14) and the relation:

$$\Sigma^+_{Bi}\Sigma_{Bi} = \sum_{\mathfrak{z}} d^+_{B\mathfrak{z}\downarrow}(R_i) d_{B\mathfrak{z}\downarrow}(R_i). \tag{5.18}$$

This relation holds provided that only low-lying eigenstates $|\psi^B_n\rangle$ are considered and overlap is neglected. In that case we can also use

$$\{\Sigma^+_{Bi}, \Sigma_{Bi}\} = \sum_{\mathfrak{z}} D^i_{B\mathfrak{z}\mathfrak{z}} = 1$$
$$D^i_{B\mathfrak{z}_1\mathfrak{z}_2} D^i_{B\mathfrak{z}_3\mathfrak{z}_4} = \delta_{\mathfrak{z}_2\mathfrak{z}_3} D^i_{B\mathfrak{z}_1\mathfrak{z}_4}. \tag{5.19}$$

Further the operators (5.15) and (5.16) satisfy the following commutation and anti-commutation relations:

$$\begin{aligned} [D^i_{B\mathfrak{z}_1\mathfrak{z}_2}, D^i_{B\mathfrak{z}_3\mathfrak{z}_4}] &= \delta_{ij}[D^i_{B\mathfrak{z}_1\mathfrak{z}_4}\delta_{\mathfrak{z}_2\mathfrak{z}_3} - D^i_{B\mathfrak{z}_3\mathfrak{z}_2}\delta_{\mathfrak{z}_1\mathfrak{z}_4}] \\ [D^i_{B\mathfrak{z}_1\mathfrak{z}_2}, \Sigma_{Bj}] &= 0 \\ [\Sigma^{(+)}_{Bi}, \Sigma_{Bj}] &= 0 \qquad (i\neq j) \\ \{\Sigma_{Bi}, \Sigma_{Bi}\} &= 0. \end{aligned} \tag{5.20}$$

Thus the operators $D^i_{B\mathfrak{z}_1\mathfrak{z}_2}$ satisfy the same relations as the operators $D^i_{\mathfrak{z}_1\mathfrak{z}_2}$, given by (4.31), i.e. the results of section 4 can be used directly as far as the interaction terms in H_{eff} are concerned. Next we rewrite the remaining terms using (5.19). Then the following expression is obtained for H_{eff}:

$$H_{\text{eff}} = E_{\text{Cl}} - \frac{\hbar^2}{8m\alpha}\sum_{i,\hat{\xi}} P^i_{B\hat{\xi}} P^i_{B\hat{\xi}} + \tfrac{1}{2}\alpha \sum_{i,j}\sum_{\hat{\xi},\hat{\eta}} M_{\hat{\xi}\hat{\eta}}(R_{ij}) S^i_{B\hat{\xi}} S^j_{B\hat{\xi}} + \sum_{M=3}^{\infty} V^B_M$$
$$+ \mathrm{i}\mu_B B \sum_i \left[S^i_{B\hat{x}} P^i_{B\hat{y}} - S^i_{B\hat{y}} P^i_{B\hat{x}} \right] + \mu_B^2 B^2 \frac{m\alpha}{\hbar^2} \sum_i \sum_{\hat{\xi}=\{\hat{x},\hat{y}\}} S^i_{B\hat{\xi}} S^i_{B\hat{\xi}}$$
$$- \mu_B B \left[2N - \sum_i 2\Sigma^+_{Bi}\Sigma_{Bi} \right] \tag{5.21}$$

where

$$V^B_M = \tfrac{1}{2}\sum_{i\neq j}\sum_{q}{}' \mathrm{e}^{\mathrm{i}q\cdot R_{ij}} \frac{4\pi e^2}{\Omega q^2} \mathrm{e}^{-\alpha q^2} \frac{1}{M!}\alpha^{M/2} \left[\mathrm{i}\sum_{\hat{\xi}} (q\cdot\hat{\xi})(S^i_{B\hat{\xi}} - S^j_{B\hat{\xi}}) \right]^M \tag{5.22}$$

and

$$S^i_{B\hat{\xi}} = \sum_{\mathfrak{z}} \sqrt{\mathfrak{z}\cdot\hat{\xi}+1}[D^i_{B\mathfrak{z}+\hat{\xi},\mathfrak{z}} + D^i_{B\mathfrak{z},\mathfrak{z}+\hat{\xi}}]$$
$$P^i_{B\hat{\xi}} = \sum_{\mathfrak{z}} \sqrt{\mathfrak{z}\cdot\hat{\xi}+1}[D^i_{B\mathfrak{z},\mathfrak{z}+\hat{\xi}} - D^i_{B\mathfrak{z}+\hat{\xi},\mathfrak{z}}]. \tag{5.23}$$

The second rank tensor $M(R_{ij})$ is given by (4.45).

In order to obtain the eigenvalues and eigenstates of the low-density electron system in a homogeneous magnetic field up to order $r_s^{-3/2}$ all higher order terms represented by V^B_M in (5.21) are neglected and the following tensor is introduced:

$$\begin{aligned} M_{\mathrm{B}}(R_{ij}) &= M(R_{ij}) \qquad i \neq j \\ M_{B\hat{\xi}\hat{\eta}}(0) &= M_{\hat{\xi}\hat{\eta}}(0) + \frac{m\mu_{\mathrm{B}}^2 B^2}{\hbar^2}[\delta_{\hat{\xi}\hat{x}}\delta_{\hat{\eta}\hat{x}} + \delta_{\hat{\xi}\hat{y}}\delta_{\hat{\eta}\hat{y}}] \\ &= \left(\frac{8\pi N e^2}{3\Omega} + \frac{m\mu_{\mathrm{B}}^2 B^2}{\hbar^2}[\delta_{\hat{\xi}\hat{x}} + \delta_{\hat{\xi}\hat{y}}]\right)\delta_{\hat{\xi}\hat{\eta}} \end{aligned} \tag{5.24}$$

In terms of the boson operators

$$A_{Bk\lambda} = \frac{1}{\sqrt{2N}}\sum_{i,\hat{\xi}}\left[\mathrm{e}^{-\mathrm{i}k\cdot R_i}\varepsilon^B_{-k\lambda}\cdot\hat{\xi}\left(\sqrt{\frac{m\omega_{Bk\lambda}\alpha}{2\hbar}}S^i_{B\hat{\xi}} + \sqrt{\frac{\hbar}{8m\omega_{Bk\lambda}\alpha}}P^i_{B\hat{\xi}}\right)\right]$$
$$A^+_{Bk\lambda} = \frac{1}{\sqrt{2N}}\sum_{i,\hat{\xi}}\left[\mathrm{e}^{\mathrm{i}k\cdot R_i}\varepsilon^B_{k\lambda}\cdot\hat{\xi}\left(\sqrt{\frac{m\omega_{Bk\lambda}\alpha}{2\hbar}}S^i_{B\hat{\xi}} - \sqrt{\frac{\hbar}{8m\omega_{Bk\lambda}\alpha}}P^i_{B\hat{\xi}}\right)\right] \tag{5.25}$$

where $\omega_{Bk\lambda}$ and $\varepsilon^B_{k\lambda}$ are given by the eigenvalue equation

$$\sum_i \mathrm{e}^{\mathrm{i}k\cdot R_i}M_{\mathrm{B}}(R_i)\varepsilon^B_{k\lambda} = m\omega^2_{Bk\lambda}\varepsilon^B_{k\lambda} \tag{5.26}$$

the effective Hamiltonian can then be expressed as

$$H_{\mathrm{eff}} = E_{\mathrm{CI}} + \sum_{k\lambda}\left[\hbar\omega_{Bk\lambda}[\tfrac{1}{2} + A^+_{Bk\lambda}A_{Bk\lambda}] + \sum_{\lambda'}\mathrm{i}\mu_{\mathrm{B}}B\cdot(\varepsilon^B_{k\lambda'}\times\varepsilon^B_{k\lambda})A^+_{Bk\lambda'}A_{Bk\lambda}\right]$$
$$-\mu_{\mathrm{B}}B\left[2N - \sum_i 2\Sigma^+_{Bi}\Sigma_{Bi}\right]. \tag{5.27}$$

This Hamiltonian consists of two different parts. The first part describes a system of non-interacting bosons, where the different polarizations λ are mixed because of the magnetic field. The second part represents a system of uncoupled paulions according to (5.19) and (5.20). Both parts commute with each other as follows from (5.20).

The boson part of Hamiltonian (5.27) is a bilinear form of the boson operators and can therefore be diagonalized by the unitary transformation

$$B_{k\mu} = \sum_\lambda u_{\lambda\mu}A_{Bk\lambda}$$
$$B^+_{k\mu} = \sum_\lambda u^*_{\lambda\mu}A^+_{Bk\lambda} \tag{5.28}$$

where

$$\sum_{\lambda} u_{\lambda\mu} u^*_{\lambda\mu'} = \delta_{\mu\mu'} \tag{5.29}$$

and

$$\sum_{\mu} u_{\lambda\mu} u^*_{\lambda'\mu} = \delta_{\lambda\lambda'}. \tag{5.30}$$

Substituting into (5.27) the inverse transformation

$$\begin{aligned} A_{Bk\lambda} &= \sum_{\mu} u^*_{\lambda\mu} B_{k\mu} \\ A^+_{Bk\lambda} &= \sum_{\mu} u_{\lambda\mu} B^+_{k\mu} \end{aligned} \tag{5.31}$$

the effective Hamiltonian can be represented as

$$H_{\text{eff}} = E_{\text{Cl}} + \tfrac{1}{2}\sum_{k\lambda} \hbar\omega_{Bk\lambda} + \sum_{k\mu} \hbar E_{k\mu} B^+_{k\mu} B_{k\mu} - \mu_{\text{B}} B \left[2N - 2\sum_i \Sigma^+_{Bi} \Sigma_{Bi} \right]. \tag{5.32}$$

The frequencies appearing, $E_{k\mu}$ and the operators $B^{(+)}_{k\mu}$ are determined by the eigenvalue equation

$$\sum_{\lambda'} \Omega^k_{\lambda\lambda'} u_{\lambda'\mu} = E_{k\mu} u_{\lambda\mu} \tag{5.33}$$

where the hermitean matrix Ω^k is given by

$$\Omega^k_{\lambda\lambda'} = \omega_{Bk\lambda}\delta_{\lambda\lambda'} + \mathrm{i}\frac{\mu_{\text{B}} B}{\hbar} \cdot (\varepsilon^B_{k\lambda'} \times \varepsilon^B_{k\lambda}). \tag{5.34}$$

The eigenvalues $E_{k\mu}$ are the solutions of the following third order algebraic equation:

$$\begin{aligned} &(E_{k\mu} - \omega_{Bk1})(E_{k\mu} - \omega_{Bk2})(E_{k\mu} - \omega_{Bk3}) \\ &\quad = \omega^2_{c23}(E_{k\mu} - \omega_{Bk1}) + \omega^2_{c31}(E_{k\mu} - \omega_{Bk2}) + \omega^2_{c12}(E_{k\mu} - \omega_{Bk3}) \end{aligned} \tag{5.35}$$

with

$$\omega_{c\lambda\lambda'} = \frac{\mu_{\text{B}} B}{\hbar} \cdot (\varepsilon^B_{k\lambda'} \times \varepsilon^B_{k\lambda}). \tag{5.36}$$

Thus the energy spectrum of the original Hamiltonian (5.1) is known up to order $r_s^{-3/2}$, as follows from the expression (5.32) which is the sum of a free boson and an uncoupled paulion system. The corresponding eigenstates are given by

$$|\psi^B_n\rangle = \prod_{k,\mu} \frac{1}{\sqrt{n_{k\mu}!}} \left(B^+_{k\mu} \right)^{n_{k\mu}} \prod_i (\Sigma^+_{Bi})^{n_i} |\psi^B_0\rangle \tag{5.37}$$

where $n_{k\mu}$ and n_i are boson and fermion occupation numbers, respectively, i.e. $n_{k\mu} = 0,1,2,3,\ldots$ and $n_i = 0,1$. The ground state $|\psi_0^B\rangle$ is obtained using the representation (5.3) and

$$\Sigma_{Bi}|\psi_0^B\rangle = B_{k\mu}|\psi_0^B\rangle = 0 \tag{5.38}$$

for all i, k and μ. As expected all spins are directed along the magnetic field in the ground state.

The thermodynamic properties at low temperatures $T = 1/k_B\beta$ follow directly from the internal energy

$$E = E_{CI} + \tfrac{1}{2}\sum_{k\lambda}\hbar\omega_{Bk\lambda} - 2N\mu_B B + \sum_{k\mu}\hbar E_{k\mu}[e^{\beta\hbar E_{k\mu}} - 1]^{-1} + 4N\mu_B B[e^{2\mu_B B\beta} + 1]^{-1}. \tag{5.39}$$

Finally we have to show that a homogeneous field in the jellium model can exist according to Maxwell's equations. This means that the response of the system to the supposed homogeneous field, i.e. the current density, must be calculated. The current density operator $\jmath(r)$, which is defined by the equation of continuity, is for the present system

$$\jmath(r) = \sum_\sigma\left[-\frac{ie\hbar}{2m}[\psi_\sigma^+(r)\nabla\psi_\sigma(r) - (\nabla\psi_\sigma^+(r))\psi_\sigma(r)] - \frac{e^2}{mc}A(r)\psi_\sigma^+(r)\psi_\sigma(r)\right] \tag{5.40}$$

where $A(r)$ is given by (5.2). Analogous to the Hamilton operator the current density operator can be replaced as well by an effective operator having the same eigenvalue spectrum as $\jmath(r)$ provided that overlap is neglected. This effective current density operator is given by

$$\jmath_{\text{eff}}(r) = \sum_i\sum_{j_1 j_2}\jmath^i_{j_1 j_2}(r)D^i_{Bj_1 j_2} \tag{5.41}$$

where

$$\jmath^i_{j_1 j_2}(r) = -\frac{ie\hbar}{2m}\left[f^{*B}_{j_1 R_i}(r-R_i)\nabla f^B_{j_2 R_i}(r-R_i) - f^B_{j_2 R_i}(r-R_i)\nabla f^{*B}_{j_1 R_i}(r-R_i)\right] - \frac{e^2}{mc}A(r)f^{*B}_{j_1 R_i}(r-R_i)f^B_{j_2 R_i}(r-R_i). \tag{5.42}$$

Substituting (5.9) into (5.42) we obtain

$$\jmath^i_{j_1 j_2}(r) = \frac{-ie\hbar}{2m}[f^*_{j_1}(r-R_i)\nabla f_{j_2}(r-R_i) - f_{j_2}(r-R_i)\nabla f^*_{j_1}(r-R_i)] - \frac{e^2}{mc}[A(r) - A(R_i)]f^*_{j_1}(r-R_i)f_{j_2}(r-R_i). \tag{5.43}$$

It should be remarked that the current density operator as given by (5.41) and (5.43) can be interpreted in terms of electrons moving around lattice sites. Hopping does not appear because overlap is neglected.

The full translational symmetry of the original Hamiltonian (5.1) implies that the current density $\mathcal{J}$ must be homogeneous as well. That quantity is obtained in the usual way by averaging the symmetry-broken thermal average $\langle \mathcal{J}_{\text{eff}}(\boldsymbol{r})\rangle$ over a unit cell of the Wigner lattice, i.e.

$$\mathcal{J} = \frac{1}{\Omega_{\text{cell}}} \int_{\text{unit cell}} \mathrm{d}^3 r \langle \mathcal{J}_{\text{eff}}(\boldsymbol{r} + \boldsymbol{R}_i)\rangle \tag{5.44}$$

where Ω_{cell} and $\boldsymbol{R}_i$ denote the volume and position of the unit cell, respectively. Substituting (5.41) into (5.44) and neglecting all terms containing $\exp[-R_{ij}^2/2\alpha]$, $i \neq j$, as they are of the order of the overlap, we obtain

$$\mathcal{J} = \frac{1}{\Omega_{\text{cell}}} \int_{\text{all space}} \mathrm{d}^3 r \sum_{\mathcal{J}_1 \mathcal{J}_2} \mathcal{J}^i_{\mathcal{J}_1 \mathcal{J}_2}(\boldsymbol{r} + \boldsymbol{R}_i) \langle D^i_{\mathcal{J}_1 \mathcal{J}_2}\rangle \tag{5.45}$$

where $\mathcal{J}^i_{\mathcal{J}_1 \mathcal{J}_2}$ is given by (5.43). Because $\langle D^i_{\mathcal{J}_1 \mathcal{J}_2}\rangle$ is invariant under lattice translations the uniform current density can now be expressed as

$$\begin{aligned}\mathcal{J} &= \frac{1}{2N} \sum_i \frac{1}{\Omega_{\text{cell}}} \int \mathrm{d}^3 r \sum_{\mathcal{J}_1 \mathcal{J}_2} \mathcal{J}^i_{\mathcal{J}_1 \mathcal{J}_2}(\boldsymbol{r}) \langle D^i_{\mathcal{J}_1 \mathcal{J}_2}\rangle = \frac{1}{\Omega} \int \mathrm{d}^3 r \langle \mathcal{J}_{\text{eff}}(\boldsymbol{r})\rangle \\ &= \frac{-\mathrm{i}e\hbar}{2m\sqrt{\alpha}\Omega} \sum_{i,\hat{\boldsymbol{\xi}}} \langle P^i_{\hat{\boldsymbol{\xi}}}\rangle \hat{\boldsymbol{\xi}} - \frac{e^2 B\sqrt{\alpha}}{2mc\Omega} \sum_i [\langle S^i_{B\hat{\boldsymbol{x}}}\rangle \hat{\boldsymbol{y}} - \langle S^i_{B\hat{\boldsymbol{y}}}\rangle \hat{\boldsymbol{x}}]\end{aligned} \tag{5.46}$$

where $S^i_{B\hat{\boldsymbol{\xi}}}$ and $P^i_{B\hat{\boldsymbol{\xi}}}$ are given by (5.23). From (5.25) and (5.31) we get

$$\begin{aligned} S^i_{B\hat{\boldsymbol{\xi}}} &= \frac{1}{\sqrt{2N}} \sum_{\boldsymbol{k},\lambda,\mu} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \sqrt{\frac{\hbar}{2m\omega_{B\boldsymbol{k}\lambda}\alpha}} [u_{\lambda\mu} B^+_{\boldsymbol{k}\mu} + u^*_{\lambda\mu} B_{-\boldsymbol{k}\mu}] \\ P^i_{B\hat{\boldsymbol{\xi}}} &= \frac{1}{\sqrt{2N}} \sum_{\boldsymbol{k},\lambda,\mu} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \sqrt{\frac{2m\omega_{B\boldsymbol{k}\lambda}\alpha}{\hbar}} [u^*_{\lambda\mu} B_{\boldsymbol{k}\mu} - u_{\lambda\mu} B^+_{-\boldsymbol{k}\mu}]. \end{aligned} \tag{5.47}$$

Substituting (5.47) into (5.46) and using that for $\boldsymbol{k} = 0$ the solutions of the eigenvalue equation (5.26) are given by

$$\begin{aligned} &m\omega^2_{B01} = m\omega^2_{B02} = \frac{8\pi N e^2}{3\Omega} + \frac{\mu_B^2 B^2 m}{\hbar^2} \qquad m\omega^2_{B03} = \frac{8\pi N e^2}{3\Omega} \\ &\boldsymbol{\varepsilon}_{01} = \hat{\boldsymbol{x}}, \boldsymbol{\varepsilon}_{02} = \hat{\boldsymbol{y}} \boldsymbol{\varepsilon}_{03} = \hat{\boldsymbol{z}} \end{aligned}$$

we arrive at

$$\begin{aligned} \mathcal{J} = \frac{\sqrt{2N}}{\Omega} \sum_\mu e\sqrt{\frac{\hbar}{2m}} \Bigg[&\left(\frac{8\pi N e^2}{3m\Omega} + \frac{\mu_B^2 B^2}{\hbar^2}\right)^{1/4} 2\mathrm{Im}(u_{1\mu}\langle B^+_{o\mu}\rangle \hat{\boldsymbol{x}} + u_{2\mu}\langle B^+_{o\mu}\rangle \hat{\boldsymbol{y}}) \\ &+ \left(\frac{8\pi N e^2}{3m\Omega}\right)^{1/4} 2\mathrm{Im}(u_{3\mu}\langle B^+_{o\mu}\rangle \hat{\boldsymbol{z}}) \\ &- \left(\frac{8\pi N e^2}{3m\Omega} + \frac{\mu_B^2 B^2}{\hbar^2}\right)^{-1/4} \frac{eB}{mc} \mathrm{Re}(u_{1\mu}\langle B^+_{o\mu}\rangle \hat{\boldsymbol{y}} - u_{2\mu}\langle B^+_{o\mu}\rangle \hat{\boldsymbol{x}}) \Bigg] \end{aligned} \tag{5.48}$$

where $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ denote the real and imaginary part of the complex number z, respectively. Clearly $\langle B^+_{o\mu}\rangle = 0$ in the free boson approximation (5.32), i.e. $\jmath = 0$. That conclusion also holds for the interacting boson system described by (5.21), as can be seen in the following way. The eigenstates required to calculate $\langle B^+_{o\mu}\rangle$ are now eigenstates of Hamiltonian (5.21). These states, when represented as linear combinations of the eigenstates $|\psi^B_n\rangle$ of the free boson Hamiltonian (5.32), have the property that they do not contain the terms $|\psi^B_n\rangle$ and $B^+_{o\mu}|\psi^B_n\rangle$ simultaneously. That property, which immediately implies $\langle B^+_{o\mu}\rangle = 0$, follows directly from the calculation of the matrix elements $\langle\psi^B_n|V^B_M B^+_{o\mu}|\psi^B_n\rangle$, which are zero due to the structure of V^B_M given by (5.22) and (5.47).

Now it can be concluded that the low-density jellium model indeed allows a homogeneous internal magnetic field. For $\jmath = 0$ and the Maxwell equations do give such a field.

5.2. Response to an inhomogeneous magnetic field

Subsection 5.1 deals with a low-density jellium model having a homogeneous internal magnetic field. The question, however, whether an external magnetic field can penetrate into the system thus creating the internal field, is not answered. For an answer to that question requires the introduction of boundaries and external field sources, which destroy the translational invariance explicitly used in subsection 5.1. The situation that a magnetic field does not penetrate a given system is known as the Meissner–Ochsenfeld effect. In order to discuss the eventual appearance of that effect in the low-density model we calculate, analogous to the procedure of the BCS-theory [17, 18], the response of the system to an inhomogeneous magnetic field. Such a field is generated by some source current density in the interior of the still infinite system.

In order to examine the possible existence of the Meissner–Ochsenfeld effect we only need to calculate the linear response of the system to the magnetic field, i.e. the linear relation between the induced current density $\jmath(\boldsymbol{r}, t)$ and the vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$. This means that the magnetic field is assumed to be very small and all terms of order $|\boldsymbol{A}|^n$, $n \geqslant 2$, are neglected.

The criterion for the appearance of the Meissner–Ochsenfeld effect is [18]

$$\lim_{q\to 0}\lim_{\omega\to 0} \jmath(\boldsymbol{q}, \omega) = -K \lim_{q\to 0}\lim_{\omega\to 0} \boldsymbol{A}(\boldsymbol{q}, \omega) \tag{5.49}$$

where K is a non-zero constant and $\jmath(\boldsymbol{q}, \omega)$ and $\boldsymbol{A}(\boldsymbol{q}, \omega)$ are given by the Fourier decompositions

$$\begin{aligned}
\boldsymbol{A}(\boldsymbol{r}, t) &= \frac{1}{\Omega}\sum_{\boldsymbol{q}} \boldsymbol{A}(\boldsymbol{q}, t)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{\Omega}\sum_{\boldsymbol{q}}\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega \boldsymbol{A}(\boldsymbol{q}, \omega)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{e}^{-\mathrm{i}\omega t} \\
\jmath(\boldsymbol{r}, t) &= \frac{1}{\Omega}\sum_{\boldsymbol{q}} \jmath(\boldsymbol{q}, t)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{\Omega}\sum_{\boldsymbol{q}}\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega \jmath(\boldsymbol{q}, \omega)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{e}^{-\mathrm{i}\omega t}.
\end{aligned} \tag{5.50}$$

The condition (5.49) is a relation between macroscopic quantities. This means in the present case that the local field and current density must be averaged over one unit cell of the Wigner lattice. It should be remarked that the resulting macroscopic quantities are no longer identical here to the microscopic ones as contrasted with the situation discussed in subsection 5.1.

Up to order $|A|$ the Hamiltonian can be expressed as

$$H = H(0) + H(1) + H_s \tag{5.51}$$

where $H(0)$ is the Hamiltonian (3.1) of the jellium model, H_s is the term describing the interaction between the electron spins and the magnetic field, and $H(1)$ is given by

$$H(1) = \frac{-\mu_B}{\Omega} \sum_{k,q} \sum_{\sigma} (2k+q) \cdot A(q,t) c^+_{k+q\sigma} c_{k\sigma}. \tag{5.52}$$

The explicit form of H_s is not given here, as H_s does not affect the current density for the following two reasons. First of all H_s commutes with the charge density operator $\rho(r) = \sum_\sigma \psi^+_\sigma(r)\psi_\sigma(r)$, i.e. H_s plays no part in the equation of continuity that determines the current density operator. Secondly the neglect of the overlap between one-electron wavefunctions localized at different lattice sites entails that the only effect of H_s on the eigenstates of $H(0)+H(1)$ is the removal of the degeneracy of these states with respect to all possible spin configurations of the lattice. Clearly then we only need to consider the Hamiltonian $\widetilde{H} = H(0) + H(1)$.

Next we replace $H(1)$ by an effective Hamiltonian $H(1)_{\text{eff}}$ analogous to the procedure discussed in section 4, i.e. we neglect the effect of exchange:

$$H(1)_{\text{eff}} = \frac{-\mu_B}{\Omega} \sum_{q,i} \sum_{j_1 j_2} e^{iq\cdot R_i} A(q,t) \cdot \left[\int d^3k (2k+q) \hat{f}^*_{j_1}(k+q) \hat{f}_{j_2}(k) \right] D^i_{j_1 j_2} \tag{5.53}$$

where $\hat{f}_j$ and $D^i_{j_1 j_2}$ are given by (4.15) and (4.31), respectively. The boson representation of this Hamiltonian is obtained in the following way. Using the relation for the Hermite polynomials,

$$(k\cdot\hat{\xi}) H_{j\cdot\hat{\xi}}(k\cdot\hat{\xi}\sqrt{2\alpha}) = \frac{1}{\sqrt{2\alpha}} \left[\tfrac{1}{2} H_{j\cdot\hat{\xi}+1}(k\cdot\hat{\xi}\sqrt{2\alpha}) + (j\cdot\hat{\xi}) H_{j\cdot\hat{\xi}-1}(k\cdot\hat{\xi}\sqrt{2\alpha}) \right] \tag{5.54}$$

we arrive at

$$\begin{aligned}
\sum_{j_1 j_2} & \left[\int d^3k (2k+q) \hat{f}^*_{j_1}(k+q) \hat{f}_{j_2}(k) \right] D^i_{j_1 j_2} \\
&= \sum_{j_1 j_2, \hat{\xi}} \frac{i\hat{\xi}}{2\sqrt{\alpha}} \left[\int d^3k \hat{f}^*_{j_1}(k+q) \hat{f}_{j_2}(k) \right] \left[\sqrt{j_1\cdot\hat{\xi}+1} (D^i_{j_1+\hat{\xi}, j_2} - D^i_{j_2, j_1+\hat{\xi}}) \right. \\
&\quad \left. + \sqrt{j_1\cdot\hat{\xi}} (D^i_{j_2, j_1-\hat{\xi}} - D^i_{j_1-\hat{\xi}, j_2}) \right] \\
&= - \sum_{j_1 j_2, \hat{\xi}} \frac{i\hat{\xi}}{2\sqrt{\alpha}} \left[\int d^3k \hat{f}^*_{j_1}(k+q) \hat{f}_{j_2}(k) \right] \left[D^i_{j_2 j_1} P^i_{\hat{\xi}} + P^i_{\hat{\xi}} D^i_{j_1 j_2} \right]
\end{aligned} \tag{5.55}$$

where $P^i_{\hat{\xi}}$ is given by (4.47) and use is made of (4.35). Next we expand the right hand side of (5.55) in terms of the components of $\sqrt{\alpha}q$. Such an expansion is explicitly

done up to fourth order in appendix 5. The resulting expression (A5.5) can be directly generalized to the following result:

$$\sum_{j_1 j_2}\left[\int \mathrm{d}^3k \hat{f}^*_{j_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{j_2}(\boldsymbol{k})\right] D^i_{j_1 j_2} = 1 + \chi_0(\boldsymbol{q}) + \sum_{M=1}^{\infty}\sum_{\hat{\xi}_1\ldots\hat{\xi}_M} \chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(\boldsymbol{q}) S^i_{\hat{\xi}_1} S^i_{\hat{\xi}_2}\ldots S^i_{\hat{\xi}_M} \tag{5.56}$$

where $S^i_{\hat{\xi}}$ is given by (4.40) and the functions χ_0 and $\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}$ satisfy

$$\lim_{\boldsymbol{q}\to 0}\chi_0(\boldsymbol{q}) = \lim_{\boldsymbol{q}\to 0}\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(\boldsymbol{q}) = 0. \tag{5.57}$$

Substitution of (5.55) and (5.56) into (5.53) gives

$$H(1)_{\mathrm{eff}} = \frac{\mu_{\mathrm{B}}\mathrm{i}}{\Omega\sqrt{\alpha}}\sum_{\boldsymbol{q},\mathrm{i},\hat{\xi}} \boldsymbol{A}(\boldsymbol{q},t)\cdot\hat{\xi}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_\mathrm{i}}\left[P^i_{\hat{\xi}}[1+\chi_0(\boldsymbol{q})] + \sum_{M=1}^{\infty}\sum_{\hat{\xi}_1\ldots\hat{\xi}_M}\tfrac{1}{2}\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(\boldsymbol{q})\left[P^i_{\hat{\xi}}S^i_{\hat{\xi}_1}\ldots S^i_{\hat{\xi}_M} + S^i_{\hat{\xi}_1}\ldots S^i_{\hat{\xi}_M}P^i_{\hat{\xi}}\right]\right]. \tag{5.58}$$

This Hamiltonian can be easily expressed in terms of the boson operators $A^{(+)}_{\boldsymbol{k}\lambda}$, using (4.51) and (4.54). The relevant Hamiltonian, $\widetilde{H} = H(0) + H(1)$, can now be replaced by the following effective Hamiltonian:

$$\widetilde{H}_{\mathrm{eff}} = H(0)_{\mathrm{eff}} + H(1)_{\mathrm{eff}} \tag{5.59}$$

where, as shown in appendix 5, $H(0)_{\mathrm{eff}}$ has the following form

$$H(0)_{\mathrm{eff}} = E_{\mathrm{Cl}} + \sum_{\boldsymbol{k}\lambda}[\tfrac{1}{2} + A^+_{\boldsymbol{k}\lambda}A_{\boldsymbol{k}\lambda}]\hbar\omega_{\boldsymbol{k}\lambda} + \sum_{M=3}^{\infty} V_M \tag{5.60}$$

with

$$V_M = N\sum_{\boldsymbol{K}_n}\sum_{\boldsymbol{R}_i\neq 0}\sum_{\boldsymbol{q}_0}{}' \mathrm{e}^{\mathrm{i}\boldsymbol{q}_0\cdot\boldsymbol{R}_i}\frac{4\pi e^2}{\Omega q_0^2}\mathrm{e}^{-\alpha q_0^2}\frac{\mathrm{i}^M}{M!}\sum_{\substack{\boldsymbol{k}_1\ldots\boldsymbol{k}_M\\ \lambda_1\ldots\lambda_M}}\delta_{\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M,\boldsymbol{K}_n} \times\prod_{j=1}^{M}\left[\sqrt{\frac{\hbar}{4Nm\omega_{\boldsymbol{k}_j\lambda_j}}}\boldsymbol{\varepsilon}_{\boldsymbol{k}_j\lambda_j}\cdot\boldsymbol{q}_0[\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{R}_i}-1][A^+_{\boldsymbol{k}_j\lambda_j}+A_{-\boldsymbol{k}_j\lambda_j}]\right] \tag{5.61}$$

whereas $H(1)_{\mathrm{eff}}$ is given by

$$H(1)_{\mathrm{eff}} = \frac{\mu_{\mathrm{B}}\mathrm{i}\sqrt{2N}}{\Omega}\sum_{\boldsymbol{K}_n}\sum_{\boldsymbol{k}\lambda}\sqrt{\frac{2m\omega_{\boldsymbol{k}\lambda}}{\hbar}}\Big\{\boldsymbol{A}(\boldsymbol{k}+\boldsymbol{K}_n,t)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \times[1+\chi_0(\boldsymbol{k}+\boldsymbol{K}_n)][A_{\boldsymbol{k}\lambda}-A^+_{-\boldsymbol{k}\lambda}]$$

$$+\tfrac{1}{2}\sum_{M=1}^{\infty}\sum_{\hat{\xi}_1\ldots\hat{\xi}_M}\sum_{k_1\ldots k_M,\lambda_1\ldots\lambda_M} A(k+K_n-(k_1+\ldots+k_M),t)\cdot\varepsilon_{k\lambda}$$
$$\times[\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(k+K_n-(k_1+\ldots+k_M))]$$
$$\times\Big[\Big(\prod_{j=1}^{M}\sqrt{\frac{\hbar}{4Nm\alpha\omega_{k_j\lambda_j}}}\varepsilon_{k_j\lambda_j}\cdot\hat{\xi}_j[A^{+}_{k_j\lambda_j}+A_{-k_j\lambda_j}]\Big)[A_{k\lambda}-A^{+}_{-k\lambda}]$$
$$+[A_{k\lambda}-A^{+}_{k\lambda}]\Big(\prod_{j=1}^{M}\sqrt{\frac{\hbar}{4Nm\alpha\omega_{k_j\lambda_j}}}\varepsilon_{k_j\lambda_j}\cdot\hat{\xi}_j[A^{+}_{k_j\lambda_j}+A_{-k_j\lambda_j}]\Big)\Big]\Big\}. \tag{5.62}$$

The summation over K_n in (5.61) and (5.62) runs over all reciprocal lattice vectors. In obtaining (5.61) and (5.62) we assumed that the origin of our coordinate system coincides with a site of the Wigner lattice. That assumption does not influence our conclusion concerning the eventual appearance of the Meissner–Ochsenfeld effect as we are only interested in the macroscopic current density.

Now we discuss an important property of the eigenstates $|\varphi_n\rangle$ of $H(0)_{\text{eff}}$ for the sake of the calculation of the current density. The states $|\varphi_n\rangle$ are linear combinations of the eigenstates $|\psi_m\rangle$ of the free boson term of (5.60). For convenience' sake this complete set of states $|\psi_m\rangle$ is divided into subsets consisting of those eigenstates $|\psi_{lK}\rangle$ that have the same total wave vector K given by

$$K=\sum_{k\lambda}n_{k\lambda}k \tag{5.63}$$

with $n_{k\lambda}=0,1,2,\ldots$ being the occupation number of the one-boson state $|k\lambda\rangle$. Because of the factor $\delta_{k_1+\ldots+k_M,K_n}$ in (5.61) the complete set of eigenstates $|\varphi_n\rangle$ of $H(0)_{\text{eff}}$ can now be divided into subsets consisting of eigenstates $|\varphi_{nK}\rangle$ satisfying

$$|\varphi_{nK}\rangle=\sum_{K_n}\sum_{l}C^{n}_{lK_n}|\psi_{lK+K_n}\rangle \tag{5.64}$$

where the summation over l runs over the subset consisting of states that have the total wave vector $K+K_n$ and the constants $C^{n}_{lK_n}$ satisfy

$$\sum_{K_n}\sum_{l}|C^{n}_{lK_n}|^2=1. \tag{5.65}$$

Thus the eigenstates $|\varphi_n\rangle$ have the following property:

$$\langle\varphi_n|\prod_j(A^{+}_{k_j\lambda_j}+\operatorname{sgn}(j)A_{-k_j\lambda_j})|\varphi_n\rangle=0 \quad \text{for} \quad \sum_j k_j\neq K_n \tag{5.66}$$

where $\operatorname{sgn}(j)=+1$ or $\operatorname{sgn}(j)=-1$ and K_n may be any reciprocal lattice vector.

The current density operator, which follows from the equation of continuity, is given by

$$\jmath(r,t)=\frac{1}{\Omega}\sum_{q}[\jmath^{P}(q,t)+\jmath^{D}(q,t)]e^{iq\cdot r} \tag{5.67}$$

where

$$\mathcal{J}^P(q,t) = \frac{e\hbar}{2m}\sum_{k\sigma}[2k+q]c^+_{k+q\sigma}c_{k\sigma} \tag{5.68}$$

and

$$\mathcal{J}^D(q,t) = \frac{-e^2}{mc\Omega}\sum_{k,q',\sigma} A(q-q',t)c_{k+q'\sigma}c_{k\sigma} \tag{5.69}$$

are the Fourier transforms of the paramagnetic and diamagnetic current density operator, respectively. The effective operators corresponding with $\mathcal{J}^P(q,t)$ and $\mathcal{J}^D(q,t)$ read

$$\mathcal{J}^P_{\text{eff}}(q,t) = \frac{e\hbar}{2m}\sum_i\sum_{j_1j_2} e^{iq\cdot R_i}\left[\int d^3k(2k+q)\hat{f}^*_{j_1}(k+q)\hat{f}_{j_2}(k)\right]D^i_{j_1j_2} \tag{5.70}$$

$$\mathcal{J}^D_{\text{eff}}(q,t) = \frac{-e^2}{mc\Omega}\sum_{i,q'}\sum_{j_1j_2} A(q-q',t)e^{iq'\cdot R_i}\left[\int d^3k\hat{f}^*_{j_1}(k+q')\hat{f}_{j_2}(k)\right]D^i_{j_1j_2}. \tag{5.71}$$

As follows from (5.49) we only need to consider $\mathcal{J}^P_{\text{eff}}(q,t)$ and $\mathcal{J}^D_{\text{eff}}(q,t)$ in the limit $q \to 0$. Using (5.55), (5.56) and (5.57) we obtain

$$\lim_{q\to 0}\mathcal{J}^P_{\text{eff}}(q,t) = \lim_{q\to 0}\left\{\frac{-ie\hbar}{2m\sqrt{\alpha}}\sum_{i,\hat{\xi}}\hat{\xi}e^{iq\cdot R_i}P^i_{\hat{\xi}}\right\} \tag{5.72}$$

$$\lim_{q\to 0}\mathcal{J}^D_{\text{eff}}(q,t) = \lim_{q\to 0}\left\{\frac{-e^2}{mc\Omega}\sum_{i,q'}A(q-q',t)e^{iq'\cdot R_i}\left[1+\chi_0(q')\right.\right.$$
$$\left.\left.+\sum_{M=1}^{\infty}\sum_{\hat{\xi}_1\ldots\hat{\xi}_M}\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(q')S^i_{\hat{\xi}_1}S^i_{\hat{\xi}_2}\ldots S^i_{\hat{\xi}_M}\right]\right\}. \tag{5.73}$$

In terms of the boson operators these expressions read

$$\lim_{q\to 0}\mathcal{J}^P_{\text{eff}}(q,t) = \lim_{q\to 0}\left\{\frac{-ie\hbar\sqrt{2N}}{2m}\sum_\lambda \varepsilon_{q\lambda}\sqrt{\frac{2m\omega_{q\lambda}}{\hbar}}[A_{q\lambda}-A^+_{-q\lambda}]\right\} \tag{5.74}$$

$$\lim_{q\to 0}\mathcal{J}^D_{\text{eff}}(q,t) = \lim_{q\to 0}\left\{\frac{-2Ne^2}{mc\Omega}\sum_{K_n}\left[A(q-K_n,t)[1+\chi_0(K_n)]\right.\right.$$
$$+\sum_{M=1}^{\infty}\sum_{\hat{\xi}_1\ldots\hat{\xi}_M}\sum_{k_1\ldots k_M,\lambda_1\ldots\lambda_M}A(q-K_n-(k_1+\ldots+k_M),t)$$
$$\left[\chi_{\hat{\xi}_1\ldots\hat{\xi}_M}(K_n+k_1+\ldots+k_M)\right.$$
$$\left.\left.\left.\times\prod_{j=1}^{M}\sqrt{\frac{\hbar}{4Nm\alpha\omega_{k_j\lambda_j}}}\varepsilon_{k_j\lambda_j}\cdot\hat{\xi}_j(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})\right]\right]\right\}. \tag{5.75}$$

The macroscopic quantity $\lim_{q\to 0} \jmath(q,\omega)$, that appears in the criterion (5.49) for the Meissner–Ochsenfeld effect, can now be calculated provided that $A(q,t)$ is interpreted as a Fourier component of the macroscopic field. This interpretation implies

$$\lim_{q\to 0} A(q+K_n,t) = 0 \qquad \text{for} \qquad K_n \neq 0. \tag{5.76}$$

The calculation goes as follows. Up to linear order in the field $A(q,t)$ the Fourier component $\jmath(q,t)$ of the macroscopic current density is given by

$$\jmath(q,t) = \jmath^P(q,t) + \jmath^D(q,t) \tag{5.77}$$

with

$$\jmath^P(q,t) = \lim_{\varepsilon\to 0} \frac{1}{i\hbar} \int_{-\infty}^{t} d\tau e^{\varepsilon\tau} \langle [\jmath^P_{\text{eff}}(q,t), H(1)_{\text{eff}}(\tau)] \rangle \tag{5.78}$$

and

$$\jmath^D(q,t) = \langle \jmath^D_{\text{eff}}(q,t) \rangle. \tag{5.79}$$

The thermal average $\langle \ldots \rangle$ is taken with respect to the eigenstates $|\varphi_n\rangle$ of $H(0)_{\text{eff}}$, i.e.

$$\langle \ldots \rangle = \left[\sum_n e^{-\beta E_n} \right]^{-1} \left[\sum_n e^{-\beta E_n} \langle \varphi_n | \ldots | \varphi_n \rangle \right] \tag{5.80}$$

with E_n being the energy corresponding with $|\varphi_n\rangle$. The expression (5.78) has been derived by Kubo [19] using linear response theory. The factor $e^{\varepsilon\tau}$ in the integrand indicates that the field is switched on adiabatically. Substituting the expressions (5.62), (5.74) and (5.75) into (5.78) and (5.79), respectively, and using (5.57), (5.66) and (5.76) we arrive at

$$\lim_{q\to 0} \jmath^P(q,t) = \lim_{q\to 0} \lim_{\varepsilon\to 0} \frac{Ne^2}{mc\Omega} \sum_{k\lambda\lambda'} \varepsilon_{q\lambda'} \hbar \sqrt{\omega_{k\lambda}\omega_{q\lambda'}} \int_{-\infty}^{\infty} d\tau e^{\varepsilon\tau} A(k,\tau) \cdot \varepsilon_{k\lambda} G_1(t-\tau) \tag{5.81}$$

where $G_1(t-\tau)$ is a retarded Green function, given by

$$G_1(t) = -\frac{i}{\hbar} \theta(t) \langle [A_{q\lambda'}(t) - A^+_{-q\lambda'}(t), A_{k\lambda} - A^+_{-k\lambda}] \rangle \tag{5.82}$$

and

$$\lim_{q\to 0} \jmath^D(q,t) = -\lim_{q\to 0} \frac{2Ne^2}{mc\Omega} A(q,t). \tag{5.83}$$

Consequently the Fourier transforms $\jmath(q,\omega)$ and $A(q,\omega)$, as given by (5.50), satisfy the following relation:

$$\lim_{q\to 0}\lim_{\omega\to 0}\jmath(q,\omega)=\lim_{q\to 0}\lim_{\omega\to 0}\lim_{\varepsilon\to 0}\frac{2Ne^2}{mc\Omega}\Big[-A(q,\omega)+\tfrac{1}{2}\sum_{k\lambda\lambda'}\varepsilon_{q\lambda'}\hbar\sqrt{\omega_{k\lambda}\omega_{q\lambda'}}A(k,\omega)G_1(\omega+\mathrm{i}\varepsilon)\Big] \tag{5.84}$$

with

$$G_1(\omega)=\int_{-\infty}^{\infty}\mathrm{d}t G_1(t)\mathrm{e}^{\mathrm{i}\omega t}. \tag{5.85}$$

The final step of the calculation consists of determining the Fourier transform $G_1(\omega)$ of the retarded Green function (5.82) in the limit $\omega\to 0$. This is done by using the equations of motion for the retarded Green functions. The relevant equations of motion are

$$\begin{aligned}\mathrm{i}\hbar\frac{dG_1(t)}{dt}&=\frac{-\mathrm{i}}{\hbar}\theta(t)\langle[[A_{q\lambda'}(t)-A^{+}_{-q\lambda'}(t),H(0)_{\mathrm{eff}}],A_{k\lambda}-A^{+}_{-k\lambda}]\rangle\\&=\hbar\omega_{q\lambda'}G_2(t)+\sum_{M=3}^{\infty}2M\Big\{N\sum_{K_n}\sum_{R_i\neq 0}\sum_{q_0}{}'\mathrm{e}^{\mathrm{i}q_0\cdot R_i}\frac{4\pi e^2}{\Omega q_0^2}\mathrm{e}^{-\alpha q_0^2}\frac{\mathrm{i}^M}{M!}\\&\quad\times\sum_{\substack{k_1\ldots k_M\\ \lambda_1\ldots\lambda_M}}\delta_{k_1+\ldots+k_M,K_n}\prod_{j=1}^{M}\Big[\sqrt{\frac{\hbar}{4Nm\omega_{k_j\lambda_j}}}\varepsilon_{k_j\lambda_j}\cdot q_0[\mathrm{e}^{-\mathrm{i}k_j\cdot R_i}-1]\Big]\\&\quad\times\delta_{k_1q}G_M(t)\Big\}\end{aligned} \tag{5.86}$$

and

$$\mathrm{i}\hbar\frac{dG_2(t)}{dt}=-2\delta(t)\delta_{-kq}\delta_{\lambda\lambda'}+\hbar\omega_{q\lambda'}G_1(t) \tag{5.87}$$

where the retarded Green functions $G_2(t)$ and $G_M(t)$ are given by

$$\begin{aligned}G_2(t)&=-\frac{\mathrm{i}}{\hbar}\theta(t)\langle[A_{q\lambda'}(t)+A^{+}_{-q\lambda'}(t),A_{k\lambda}-A^{+}_{-k\lambda}]\rangle\\G_M(t)&=-\frac{\mathrm{i}}{\hbar}\theta(t)\langle[\prod_{j=2}^{M}(A^{+}_{k_j\lambda_j}+A_{-k_j\lambda_j})(t),A_{k\lambda}-A^{+}_{-k\lambda}]\rangle.\end{aligned} \tag{5.88}$$

The corresponding relations between the Fourier transforms $G_1(\omega)$, $G_2(\omega)$ and $G_M(\omega)$ can easily be calculated. Eliminating $G_2(\omega)$ we arrive at

$$\begin{aligned}G_1(\omega)=\frac{1}{\hbar[\omega^2-\omega_{q\lambda}^2]}\Big[&-2\omega_{q\lambda}\delta_{-kq}\delta_{\lambda\lambda'}+\omega\sum_{M=3}^{\infty}2M\\&\times\Big\{N\sum_{K_n}\sum_{R_i\neq 0}\sum_{q_0}{}'\mathrm{e}^{\mathrm{i}q_0\cdot R_i}\frac{4\pi e^2}{\Omega q_0^2}\mathrm{e}^{-\alpha q_0^2}\frac{\mathrm{i}^M}{M!}\sum_{\substack{k_1\ldots k_M\\ \lambda_1\ldots\lambda_M}}\delta_{k_1+\ldots+k_M,K_n}\\&\times\prod_{j=1}^{M}\Big[\sqrt{\frac{\hbar}{4Nm\omega_{k_j\lambda_j}}}\varepsilon_{k_j\lambda_j}\cdot q_0[\mathrm{e}^{-\mathrm{i}k_j\cdot R_i}-1]\Big]\delta_{k_1q}G_M(\omega)\Big\}\Big].\end{aligned} \tag{5.89}$$

The Fourier transform $G_M(\omega)$ of the Green function $G_M(t)$, given by (5.88), is a very complicated function of ω. A formal expression, however, can be obtained from (5.80):

$$G_M(\omega+i\varepsilon)=\frac{1}{\hbar}\left[\sum_n e^{-\beta E_n}\right]^{-1}\left[\sum_{n,m} e^{-\beta E_n}\left\{\langle\varphi_n|\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})\right.\right.$$
$$\times|\varphi_m\rangle\langle\varphi_m|A_{k\lambda}-A^+_{-k\lambda}|\varphi_n\rangle\left[\omega+i\varepsilon+\frac{E_n-E_m}{\hbar}\right]^{-1}$$
$$-\langle\varphi_n|A_{k\lambda}-A^+_{-k\lambda}|\varphi_m\rangle\langle\varphi_m|\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})|\varphi_n\rangle$$
$$\left.\left.\times\left[\omega+i\varepsilon+\frac{E_m-E_n}{\hbar}\right]^{-1}\right\}\right] \tag{5.90}$$

where use is made of the identities

$$\langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})(t)\right]\left[A_{k\lambda}-A^+_{-k\lambda}\right]|\varphi_n\rangle$$
$$=\sum_m\langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})(t)\right]|\varphi_m\rangle\langle\varphi_m|A_{k\lambda}-A^+_{-k\lambda}|\varphi_n\rangle$$
$$=\sum_m e^{i(\frac{E_n-E_m}{\hbar})t}\langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})\right]|\varphi_m\rangle\langle\varphi_m|A_{k\lambda}-A^+_{-k\lambda}|\varphi_n\rangle \tag{5.91}$$

and

$$-i\int_{-\infty}^{\infty}dt\,\theta(t)e^{i(\omega+i\varepsilon)t}e^{i(\frac{E_n-E_m}{\hbar})t}=\left[\omega+i\varepsilon+\frac{E_n-E_m}{\hbar}\right]^{-1}. \tag{5.92}$$

After rewriting (5.90) as

$$G_M(\omega+i\varepsilon)=\frac{1}{\hbar}\left[\sum_n e^{-\beta E_n}\right]^{-1}\left[\sum_{n,m}\left[e^{-\beta E_n}-e^{-\beta E_m}\right]\right.$$
$$\left\{\langle\varphi_n|\prod_{j=2}^{M}(A^+_{k_j\lambda_j}+A_{-k_j\lambda_j})|\varphi_m\rangle\langle\varphi_m|A_{k\lambda}-A^+_{-k\lambda}|\varphi_n\rangle\right.$$
$$\left.\left.\times\left[\omega+i\varepsilon+\frac{E_n-E_m}{\hbar}\right]^{-1}\right\}\right] \tag{5.93}$$

we obtain

$$\lim_{\omega\to0}\lim_{\varepsilon\to0}(\omega+i\varepsilon)G_M(\omega+i\varepsilon)=0. \tag{5.94}$$

Substituting (5.89) and (5.94) into (5.84) we finally arrive at the decisive relation between $\jmath(q,\omega)$ and $A(q,\omega)$:

$$\lim_{q\to 0}\lim_{\omega\to 0}\jmath(q,\omega) = \lim_{q\to 0}\lim_{\omega\to 0}\frac{2Ne^2}{mc\Omega}\Big[-A(q,\omega)+A(-q,\omega)\Big]$$
$$= -\lim_{q\to 0}\lim_{\omega\to 0}\frac{2Ne^2}{mc\Omega}\Big[2\mathrm{i}\,\mathrm{Im}(A(q,\omega))\Big]. \qquad (5.95)$$

Now we can directly conclude that the low-density electron system does not show a Meissner–Ochsenfeld effect as the imaginary part of $A(q,\omega)$ disappears in the limit $q \to 0$.

We wish to remark that the present conclusion only holds for sufficiently low densities where the effect of exchange can be neglected. This neglect, however, does not automatically mean that the appearance of a Meissner–Ochsenfeld effect could be excluded a priori, for the ground state of the low-density system is highly correlated. Apparently the electron–electron correlation, which is described by the effective Hamiltonian $\widetilde{H}_{\mathrm{eff}}$ given by (5.59), does not give the necessary rigidity to the system's wave function for resisting the magnetic field [20]. This absence of sufficient rigidity in the low-density system does not follow *a priori* from a general argument, as far as we know. Likewise the effect of the exchange on the rigidity cannot be predicted. Consequently the question is still open whether the model shows a Meissner–Ochsenfeld effect at higher densities.

6. Conclusions

In this paper the low-density electron system has been studied within a purely quantum mechanical context. It appears that the semi classical approaches of Wigner and Carr can be justified. The results of Wigner's approach of the low-density electron system are identical to those of a Hartree–Fock theory with the ground state being a Slater determinant of $2N$ harmonic oscillator ground state functions localized at the sites of a regular lattice (section 3). The effect of exchange has been considered as well leading to the conclusion that a ferromagnetic lattice is favourable to an antiferromagnetic lattice for $r_s \geqslant 14$.

In order to reproduce the results of Carr's approach the quantum mechanical calculation must take into account the effect of electron–electron correlation (section 4). Now the eigenstates are expressed as linear combinations of all possible Slater determinants of $2N$ harmonic oscillator eigenfunctions, localized at the sites of the Wigner lattice. An important result of the theory is the existence of an effective free boson Hamiltonian generating the exact eigenstates and energy spectrum up to order $r_s^{-3/2}$. The appearing boson operators have been expressed completely in terms of the original fermion operators.

The implications of the approach, as developed in section 4, are not restricted to the low-density electron system only. Any lattice of atoms or ions can be treated in exactly the same way as the Wigner lattice of electrons. The results, obtained by neglecting the effect of exchange, are then identical to those of Born's lattice theory. Thus we have completely justified Born's lattice theory from a quantum mechanical point of view.

Finally the approach of section 4 has been applied to the jellium model in a magnetic field (section 5). By way of calculating the current density we have shown that the low-density jellium model allows a homogeneous internal magnetic field. The eventual appearance of a Meissner–Ochsenfeld effect has also been discussed, the conclusion being negative for a low-density system.

Appendix 1

Substitution of (3.7) into (3.4) gives the Hartree–Fock energy of the Wigner lattice

$$E_{\mathrm{HF}} = |C|^2\langle|d_{\tau_{2N}}(\boldsymbol{R}_{2N})\ldots d_{\tau_1}(\boldsymbol{R}_1)H d^+_{\tau_1}(\boldsymbol{R}_1)\ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle \tag{A1.1}$$

with

$$|C|^{-2} = \langle|d_{\tau_{2N}}(\boldsymbol{R}_{2N})\ldots d_{\tau_1}(\boldsymbol{R}_1)d^+_{\tau_1}(\boldsymbol{R}_1)\ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle. \tag{A1.2}$$

In order to calculate E_{HF} explicitly we use

$$\begin{aligned} &H d^+_{\tau_1}(\boldsymbol{R}_1)\ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle \\ &\quad = \sum_{i=1}^{2N} d^+_{\tau_1}(\boldsymbol{R}_1)\ldots d^+_{\tau_{i-1}}(\boldsymbol{R}_{i-1})[H, d^+_{\tau_i}(\boldsymbol{R}_i)]d^+_{\tau_{i+1}}(\boldsymbol{R}_{i+1})\ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle \end{aligned} \tag{A1.3}$$

whose validity directly follows from $H|\rangle = 0$. Next we rewrite (A1.3) as

$$\begin{aligned} &H d^+_{\tau_1}(\boldsymbol{R}_1)\ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle \\ &\quad = \sum_{i=1}^{2N}\sum_{j=i+1}^{2N}(-1)^{-i+j+1}\Big(\prod_{m\neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)\{[H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j)\}|\rangle \\ &\qquad + \sum_{i=1}^{2N}(-1)^{2N-i}\Big(\prod_{m\neq i} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)[H, d^+_{\tau_i}(\boldsymbol{R}_i)]|\rangle. \end{aligned} \tag{A1.4}$$

Substituting (A1.4) into (A1.1) and using

$$\begin{aligned} d_{\tau_{2N}}(\boldsymbol{R}_{2N})\ldots d_{\tau_1}(\boldsymbol{R}_1) &= (-1)^{2N-i}d_{\tau_i}(\boldsymbol{R}_i)\Big(\prod_{m\neq i} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)^+ \\ &= (-1)^{i-j-1}d_{\tau_j}(\boldsymbol{R}_j)d_{\tau_i}(\boldsymbol{R}_i)\Big(\prod_{m\neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)^+ \end{aligned} \tag{A1.5}$$

we arrive at

$$\begin{aligned} E_{\mathrm{HF}} = |C|^2 &\sum_{i=1}^{2N}\langle|d_{\tau_i}(\boldsymbol{R}_i)\Big(\prod_{m\neq i} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)^+\Big(\prod_{m\neq i} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)[H, d^+_{\tau_i}(\boldsymbol{R}_i)]|\rangle \\ &+ |C|^2\sum_{i=1}^{2N}\sum_{j=i+1}^{2N}\langle|d_{\tau_j}(\boldsymbol{R}_j)d_{\tau_i}(\boldsymbol{R}_i)\Big(\prod_{m\neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)^+ \\ &\times\Big(\prod_{m\neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m)\Big)\{[H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j)\}|\rangle. \end{aligned} \tag{A1.6}$$

Now Wick's theorem can directly be applied to this expression, as the following relations hold:

$$[H, d^+_{\tau_i}(\boldsymbol{R}_i)]|\rangle = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{f}^*(\boldsymbol{k}) c^+_{\boldsymbol{k}\tau_i}|\rangle \tag{A1.7}$$

$$\{[H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j)\} = \frac{(2\pi)^3}{\Omega} \sum_{\boldsymbol{q}}{}' \sum_{\boldsymbol{k},\boldsymbol{k}'} V(\boldsymbol{q}) \hat{f}^*(\boldsymbol{k}-\boldsymbol{q}) \hat{f}^*(\boldsymbol{k}'+\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{R}_i} \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}'+\boldsymbol{q})\boldsymbol{R}_j} c^+_{\boldsymbol{k}\tau_i} c^+_{\boldsymbol{k}'\tau_j}. \tag{A1.8}$$

The resulting expression for E_{HF} is given by

$$\begin{aligned} E_{\mathrm{HF}} = |C|^2 \sum_{\lambda} \mathrm{sgn}(\lambda) \sum_{i=1}^{2N} \delta_{\tau_i \tau_{\lambda(i)}} K(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) \prod_{m\neq i} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \\ + |C|^2 \sum_{\lambda} \mathrm{sgn}(\lambda) \tfrac{1}{2} \sum_{i\neq j} \delta_{\tau_i \tau_{\lambda(i)}} \delta_{\tau_j \tau_{\lambda(j)}} \\ \times \left[P(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}; \boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)}; \boldsymbol{R}_i - \boldsymbol{R}_j) \prod_{m\neq i} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \right] \end{aligned} \tag{A1.9}$$

with

$$|C|^{-2} = \sum_{\lambda} \mathrm{sgn}(\lambda) \prod_{m} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \tag{A1.10}$$

where the sum over λ runs over all $(2N)!$ permutations of $1, 2, \ldots, 2N$. The function S denotes the overlap, whereas the functions K and P are related to the kinetic and potential energy respectively:

$$S(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) = \{d_\uparrow(\boldsymbol{R}_{\lambda(i)}), d^+_\uparrow(\boldsymbol{R}_i)\} = \int \mathrm{d}^3 k \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})} \tag{A1.11}$$

$$K(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) = \langle |d_\uparrow(\boldsymbol{R}_{\lambda(i)})[H, d^+_\uparrow(\boldsymbol{R}_i)]|\rangle = \int \mathrm{d}^3 k \frac{\hbar^2 k^2}{2m} \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})} \tag{A1.12}$$

$$\begin{aligned} P(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}; \boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)}; \boldsymbol{R}_i - \boldsymbol{R}_j) &= \langle |d_\downarrow(\boldsymbol{R}_{\lambda(j)}) d_\uparrow(\boldsymbol{R}_{\lambda(i)}) \{[H, d^+_\uparrow(\boldsymbol{R}_i)], d^+_\downarrow(\boldsymbol{R}_j)\}|\rangle \\ &= \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \left[\int \mathrm{d}^3 k \mathrm{d}^3 k' \hat{f}^*(\boldsymbol{k}' + \boldsymbol{q}) \hat{f}^*(\boldsymbol{k} - \boldsymbol{q}) \hat{f}(\boldsymbol{k}) \hat{f}(\boldsymbol{k}') \right. \\ &\quad \left. \times \mathrm{e}^{-\mathrm{i}\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'(\boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)})} \right]. \end{aligned} \tag{A1.13}$$

Up to order $S(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})^2$ only two terms, appearing in the sum over the permutations, are relevant. The first term corresponds with the identity permutation ($\lambda(i) = i$ for all i) and the second term with the sum over all permutations of the

form $\lambda(i) = j$, $\lambda(j) = i$, $i \neq j$. Neglecting the remaining terms, i.e. considering only two-particle exchange contributions, we obtain

$$\begin{aligned} E_{\mathrm{HF}} = |C|^2 \Big\{ & \sum_i S(0)^{2N-1} K(0) + \tfrac{1}{2} \sum_{i \neq j} S(0)^{2N-2} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) \\ & - \Big[\sum_i \sum_{j \neq i} \delta_{\tau_i \tau_j} S(0)^{2N-2} [K(\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_i) \\ & + \tfrac{1}{2} P(\boldsymbol{R}_i - \boldsymbol{R}_j; \boldsymbol{R}_j - \boldsymbol{R}_i; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\ & + \sum_i \sum_{j \neq i} \sum_{m \neq i,j} \tfrac{1}{2} S(0)^{2N-3} [K(0) S(\boldsymbol{R}_j - \boldsymbol{R}_m)^2 \delta_{\tau_m \tau_j} \\ & + \delta_{\tau_i \tau_m} S(\boldsymbol{R}_m - \boldsymbol{R}_i) P(\boldsymbol{R}_i - \boldsymbol{R}_m; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) \\ & + \delta_{\tau_j \tau_m} S(\boldsymbol{R}_m - \boldsymbol{R}_j) P(0; \boldsymbol{R}_j - \boldsymbol{R}_m; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\ & + \sum_i \sum_{j \neq i} \sum_{m \neq i,j} \sum_{n \neq m,i,j} \tfrac{1}{4} \delta_{\tau_m \tau_n} S(0)^{2N-4} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 \\ & \times P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) \Big] \Big\} \end{aligned} \tag{A1.14}$$

where

$$\begin{aligned} |C|^2 &= \Big[S(0)^{2N} - \tfrac{1}{2} \sum_m \sum_{n \neq m} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 S(0)^{2N-2} \delta_{\tau_m \tau_n} \Big]^{-1} \\ &= S(0)^{2N} + \tfrac{1}{2} \sum_m \sum_{n \neq m} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 S(0)^{2N-2} \delta_{\tau_m \tau_n}. \end{aligned} \tag{A1.15}$$

Thus the first term in the expansion is

$$E_{\mathrm{HF}}(0) = 2NK(0) + \tfrac{1}{2} \sum_{i \neq j} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) \tag{A1.16}$$

where we have used that $S(0) = 1$. This expression, together with (A1.12) and (A1.13), gives the Hartree energy (3.14). The next term is of order $S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2$ and given by

$$\begin{aligned} \Delta E_{\mathrm{HF}} = \sum_i \sum_{j \neq i} & \delta_{\tau_i \tau_j} [K(0) S(\boldsymbol{R}_j - \boldsymbol{R}_i)^2 - K(\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_i) \\ & + \tfrac{1}{2} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 - \tfrac{1}{2} P(\boldsymbol{R}_i - \boldsymbol{R}_j; \boldsymbol{R}_j - \boldsymbol{R}_i; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\ & + \tfrac{1}{2} \sum_i \sum_j \sum_{m \neq i,j} [\delta_{\tau_i \tau_m} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_i - \boldsymbol{R}_m)^2 \\ & - \delta_{\tau_i \tau_m} P(\boldsymbol{R}_i - \boldsymbol{R}_m; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_m - \boldsymbol{R}_i) \\ & + \delta_{\tau_j \tau_m} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_m)^2 \\ & - \delta_{\tau_j \tau_m} P(0; \boldsymbol{R}_j - \boldsymbol{R}_m; \boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_m - \boldsymbol{R}_j)]. \end{aligned} \tag{A1.17}$$

The magnitude of ΔE_{HF} depends on the spin configuration of the electron lattice. For a ferromagnetic spin state, i.e. $\tau_n = \uparrow$ or $\tau_n = \downarrow$ for all $n = 1, 2, \ldots, 2N$ we get

$$\Delta E_{\mathrm{HF}}^{\mathrm{f}} = \sum_{\boldsymbol{R}_n \neq 0} 2N [K(0) S(\boldsymbol{R}_n)^2 - K(\boldsymbol{R}_n) S(\boldsymbol{R}_n)$$

$$- \tfrac{1}{2}P(\boldsymbol{R}_n;-\boldsymbol{R}_n;\boldsymbol{R}_n) + \tfrac{1}{2}P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_n)^2]$$
$$+ \sum_{\boldsymbol{R}_n\neq 0}\sum_{\boldsymbol{R}_m\neq \boldsymbol{R}_n,0} 2N[P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)]. \tag{A1.18}$$

For an antiferromagnetic spin state, i.e. $\tau_n = \uparrow$ for all electrons localized at the sublattice sites $\boldsymbol{R}_n$ ($n = 1,\ldots,N$) and $\tau_n = \downarrow$ for all electrons localized at $\boldsymbol{R}_n + \delta$ ($n = 1,\ldots,N$), ΔE_{HF} is given by

$$\Delta E^{\mathrm{a}}_{\mathrm{HF}} = \sum_{\boldsymbol{R}_n\neq 0} 2N[K(0)S(\boldsymbol{R}_n)^2 - K(\boldsymbol{R}_n)S(\boldsymbol{R}_n)$$
$$- \tfrac{1}{2}P(\boldsymbol{R}_n;-\boldsymbol{R}_n;\boldsymbol{R}_n) + \tfrac{1}{2}P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_n)^2]$$
$$+ \sum_{\boldsymbol{R}_n\neq 0}\sum_{\boldsymbol{R}_m\neq \boldsymbol{R}_n,0} 2N[P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)]$$
$$+ \sum_{\boldsymbol{R}_n}\sum_{\boldsymbol{R}_m\neq 0} 2N[P(0;0;\boldsymbol{R}_n+\delta)S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m;0;\boldsymbol{R}_n+\delta)S(\boldsymbol{R}_m)]. \tag{A1.19}$$

The unknown wavefunction $\hat{f}$, that appears in (A1.11), (A1.12) and (A1.13), is determined by the minimization procedure as discussed in section 3. Using the resulting Gaussian wave packet (3.16) we obtain

$$S(\boldsymbol{R}_n) = \mathrm{e}^{-R_n^2/8\alpha} \tag{A1.20}$$

$$K(\boldsymbol{R}_n) = \frac{\hbar^2}{2m}\left[\frac{3}{4\alpha} - \frac{R_n^2}{16\alpha^2}\right]\mathrm{e}^{-R_n^2/8\alpha} \tag{A1.21}$$

$$P(\boldsymbol{R}_m;0;\boldsymbol{x}) = P(0;\boldsymbol{R}_m;-\boldsymbol{x}) = \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}-\frac{1}{2}\boldsymbol{R}_m)}\mathrm{e}^{-R_n^2/8\alpha} \tag{A1.22}$$

$$P(\boldsymbol{R}_n;-\boldsymbol{R}_n;\boldsymbol{R}_n) = \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}\mathrm{e}^{-R_n^2/8\alpha}. \tag{A1.23}$$

The ferromagnetic and antiferromagnetic exchange energies are then given by

$$\Delta E^{\mathrm{f}}_{\mathrm{HF}} = 2N\sum_{\boldsymbol{R}_n\neq 0}\mathrm{e}^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}(\mathrm{e}^{\frac{1}{2}\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_n} - \tfrac{1}{2} - \tfrac{1}{2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_n})\right.$$
$$\left. + \sum_{\boldsymbol{R}_m\neq 0}\sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_m} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_m)})\right] \tag{A1.24}$$

$$\Delta E^{\mathrm{a}}_{\mathrm{HF}} = 2N\sum_{\boldsymbol{R}_n\neq 0}\mathrm{e}^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + \sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}(\mathrm{e}^{\frac{1}{2}\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_n} - \tfrac{1}{2} - \tfrac{1}{2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_n})\right.$$
$$+ \sum_{\boldsymbol{R}_m\neq 0}\sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_m} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n)})$$
$$\left. + \sum_{\boldsymbol{R}_m}\sum_{\boldsymbol{q}}{}' V(\boldsymbol{q})\mathrm{e}^{-\alpha q^2}(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_m+\delta)} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_m+\delta-\frac{1}{2}\boldsymbol{R}_n)})\right]. \tag{A1.25}$$

After performing the sums over $\boldsymbol{R}_m$ we arrive at the expressions (3.25) and (3.26) respectively.

Appendix 2

The functional $E_H(f)$, as given in (3.14), can be rewritten as

$$E_H(f) = 2N \int d^3k \frac{\hbar^2 k^2}{2m} \hat{f}(k)\hat{f}^*(k) + \tfrac{1}{2} \sum_{m \neq n} U(\boldsymbol{R}_n - \boldsymbol{R}_m) - \lim_{q \to 0} 2N^2 \tilde{V}(q) \tag{A2.1}$$

where

$$\tilde{V}(q) = \frac{4\pi e^2}{\Omega q^2} \left[\int d^3k \hat{f}(k+q)\hat{f}^*(k) \right]^2 \tag{A2.2}$$

and

$$U(\boldsymbol{R}_n - \boldsymbol{R}_m) = \sum_q \tilde{V}(q) \exp[iq \cdot (\boldsymbol{R}_n - \boldsymbol{R}_m)]. \tag{A2.3}$$

This expression can be easily minimized provided that $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ is replaced by the true Coulomb potential. Then (A2.1) reads

$$E_H(f) = E_{Cl} + 2N \left\{ \int d^3k \hat{f}(k)\hat{f}^*(k) \frac{\hbar^2 k^2}{2m} - N \lim_{q \to 0} \frac{4\pi e^2}{\Omega q^2} \left(\left[\int d^3k \hat{f}(k+q)\hat{f}^*(k) \right]^2 - 1 \right) \right\} \tag{A2.4}$$

where the energy of the classical electron gas, E_{Cl}, is given by

$$E_{Cl} = \tfrac{1}{2} \sum_{m \neq n} \frac{e^2}{|\boldsymbol{R}_m - \boldsymbol{R}_n|} - \frac{N}{\Omega} \lim_{q \to 0} \frac{4\pi e^2}{q^2} = \frac{2\pi e^2}{\Omega} \sum_q{}' \sum_{m \neq n} \frac{1}{q^2} \exp[iq \cdot (\boldsymbol{R}_m - \boldsymbol{R}_n)]. \tag{A2.5}$$

It follows from the form of the expression (A2.4) that $E_H(f)$ is minimized by a real and isotropic function. Consequently we can use the expansion:

$$\begin{aligned} \hat{f}(k+q) &= \hat{f}(k) + q \cdot \nabla \hat{f}(k) + \tfrac{1}{2}(q \cdot \nabla)^2 \hat{f}(k) + \dots \\ &= \hat{f}(k) + \frac{q \cdot k}{k} \hat{f}'(k) + \tfrac{1}{2} \left\{ \frac{(q \cdot k)^2}{k^2} \hat{f}''(k) + \hat{f}'(k) \left[\frac{q^2}{k} - \frac{(q \cdot k)^2}{k^3} \right] \right\} + \dots \end{aligned} \tag{A2.6}$$

with $\hat{f}'(k) = d\hat{f}/dk$ and $\hat{f}''(k) = d^2\hat{f}/dk^2$. Substituting (A2.6) into (A2.4) and using

$$\lim_{q \to 0} \frac{4\pi e^2}{\Omega q^2} \left\{ \left[\int d^3k \hat{f}(k+q)\hat{f}^*(k) \right]^2 - 1 \right\} = \frac{16\pi e^2}{3\Omega} \int_0^\infty k^2 dk [\hat{f}''(k) + \frac{2}{k} \hat{f}'(k)] \hat{f}(k) \tag{A2.7}$$

we arrive at

$$E_H(f) = E_{CI} + 2N\left\{4\pi\int_0^\infty k^2 \mathrm{d}k\hat{f}(k)\left[\hat{f}(k)\frac{\hbar^2k^2}{2m} - \frac{4\pi e^2N}{3\Omega}(\hat{f}''(k) + \frac{2}{k}f'(k))\right]\right.$$
$$\left. - \lambda\left[4\pi\int_0^\infty k^2\mathrm{d}k\hat{f}(k)^2 - 1\right]\right\} \tag{A2.8}$$

where the Lagrange multiplier λ has been introduced in order to take into account the normalization of $\hat{f}$. The function $\hat{f}$ is now determined by the Euler equation

$$\frac{\mathrm{d}^2}{\mathrm{d}k^2}\left(\frac{\partial\mathcal{L}}{\partial\hat{f}''}\right) - \frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{\partial\mathcal{L}}{\partial\hat{f}'}\right) + \frac{\partial\mathcal{L}}{\partial\hat{f}} = 0 \tag{A2.9}$$

where

$$\mathcal{L} = 4\pi\left[\left(-\lambda k^2 + \frac{\hbar^2k^4}{2m}\right)\hat{f}^2 - \frac{4\pi Ne^2}{3\Omega}\left(\hat{f}'' + \frac{2\hat{f}'}{k}\right)k^2\hat{f}\right]. \tag{A2.10}$$

This means that f complies with the differential equation

$$\frac{4\pi}{3}\frac{Ne^2}{\Omega}\frac{\mathrm{d}^2}{\mathrm{d}k^2}(k\hat{f}) = \left[\frac{\hbar^2k^2}{2m} - \lambda\right](k\hat{f}). \tag{A2.11}$$

The normalized solution of (A2.11) reads

$$\hat{f}_0(k) = \left[\frac{2\alpha}{\pi}\right]^{3/4}\mathrm{e}^{-\alpha k^2} \tag{A2.12}$$

and the Lagrange multiplier is given by

$$\lambda = \frac{8\pi Ne^2\alpha}{\Omega} \tag{A2.13}$$

with

$$\alpha^2 = \frac{3\Omega}{32\pi N}\frac{\hbar^2}{me^2}. \tag{A2.14}$$

The real space wavefunction f_0, which is the Fourier transform of (A2.12), is given in (3.16).

It should be remarked that the approximation of replacing $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ by the true Coulomb potential can be justified starting from the wavefunction (A2.12). Substitution of this function into the real expression for $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ gives

$$U(\boldsymbol{R}_n - \boldsymbol{R}_m) = \sum_q \frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}\mathrm{e}^{\mathrm{i}q(\boldsymbol{R}_n - \boldsymbol{R}_m)}$$
$$= \frac{e^2}{|\boldsymbol{R}_n - \boldsymbol{R}_m|}\left[1 - \mathrm{erfc}\left(\frac{|\boldsymbol{R}_n - \boldsymbol{R}_m|}{2\sqrt{\alpha}}\right)\right] \tag{A2.15}$$

where erfc is the complement of the error function. As $\mathrm{efc}(x) \simeq \mathrm{e}^{-x^2}$ for $x \to \infty$, the difference between $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ and the Coulomb potential is of the order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$, where the overlap $S(\boldsymbol{R}_n - \boldsymbol{R}_m)$ is given in (3.22). Consequently the replacement does not affect $E_{\mathrm{H}}(f)$ provided that all terms of the order of the overlap can be neglected. The minimum of $E_{\mathrm{H}}(f)$ can easily be found by substituting (A2.12) into (A2.8) and reads:

$$E_{\mathrm{H}}^{(0)} = E_{\mathrm{Cl}} + 2N\lambda. \tag{A2.16}$$

Next we minimize the Hartree–Fock energy up to order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$ starting from the expression

$$E_{\mathrm{HF}}(f) = E_{\mathrm{H}}(f) + \Delta E_{\mathrm{HF}}(f) \tag{A2.17}$$

where $E_{\mathrm{H}}(f)$ and $\Delta E_{\mathrm{HF}}(f)$ are given by (A2.1) and (A1.17) respectively. With the aid of the complete set of harmonic oscillator eigenfunctions $\hat{f}_j$ we can express the variational function $\hat{f}$ as

$$\hat{f}(\boldsymbol{k}) = \hat{f}_0(k) + \sum_{j\neq 0} A_j \hat{f}_j(\boldsymbol{k}) \tag{A2.18}$$

where $\hat{f}_0(k)$ is given by (A2.12), and the coefficients A_j are variational parameters. We remark here that $\hat{f}$ is normalized up to order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$, as will be clear from the following. Substituting (A2.18) into (A2.17) and using the orthogonality of the functions $\hat{f}_j$, $E_{\mathrm{HF}}(f)$ can be written in the following form

$$E_{\mathrm{HF}}(f) = E_{\mathrm{HF}}(f_0) + 2N \sum_{j\neq 0} [C_j |A_j|^2 - \Delta C_j (A_j + A_j^*)] \tag{A2.19}$$

with $E_{\mathrm{HF}}(f_0)$ given by (3.27), (3.28) and (3.29), whereas C_j and ΔC_j are constants of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^0$ and $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$ respectively. Minimizing $E_{\mathrm{HF}}(f)$ with respect to A_j we get

$$\begin{aligned} A_j &= \frac{\Delta C_j}{C_j} \\ E_{\mathrm{HF}}(f) &= E_{\mathrm{HF}}(f_0) - 2N \sum_{j\neq 0} \frac{\Delta C_j^2}{C_j}. \end{aligned} \tag{A2.20}$$

Thus the function that minimizes $E_{\mathrm{HF}}(f)$ consists of (A2.12) and terms of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$. It follows directly from (A2.21) that the contribution of these correction terms to $E_{\mathrm{HF}}(f)$ is of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^4$. Consequently $E_{\mathrm{HF}}(f_0)$ is the correct minimum of $E_{\mathrm{HF}}(f)$ up to order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$. The constants C_j and ΔC_j can in principle be calculated exactly. In section 3, however, we restrict ourselves to an approximate calculation as the precise form of the wavefunction seems of little interest.

Appendix 3

Consider the following sum over reciprocal lattice vectors

$$E = \sum_{K_n \neq 0} V_\alpha(K_n) e^{iK_n \cdot a} \tag{A3.1}$$

where a is an arbitrary vector and the function V_α depends on the variational parameter α as introduced in section 3. After Ewald the parameter β is introduced and E is rewritten as

$$E = \sum_{K_n} [V_\alpha(K_n) - V_\beta(K_n)] e^{iK_n \cdot a} - \lim_{q \to 0} [V_\alpha(q) - V_\beta(q)] + \sum_{K_n \neq 0} V_\beta(K_n) e^{iK_n \cdot a}. \tag{A3.2}$$

Next we substitute into (A3.2) the Fourier decomposition

$$V_\alpha(K_n) = \frac{1}{\Omega} \int d^3 r U_\alpha(r) e^{-iK_n \cdot r} \tag{A3.3}$$

with

$$U_\alpha(r) = \sum_q V_\alpha(q) e^{iq \cdot r} = \frac{\Omega}{(2\pi)^3} \int d^3 q V_\alpha(q) e^{iq \cdot r}. \tag{A3.4}$$

Using the identity

$$\sum_{K_n} e^{-iK_n(r-a)} = \frac{\Omega}{2N} \sum_{R_n} \delta^3(r - a - R_n) \tag{A3.5}$$

where R_n denotes a lattice vector ($n = 1, 2, \ldots, 2N$), we then obtain

$$E = \frac{1}{2N} \sum_{R_n} [U_\alpha(R_n + a) - U_\beta(R_n + a)] - \lim_{q \to 0} [V_\alpha(q) - V_\beta(q)] + \sum_{K_n \neq 0} V_\beta(K_n) e^{iK_n \cdot a}. \tag{A3.6}$$

Substitution of (3.24) into (A3.6) results into

$$E = \frac{1}{2N} \sum_{R_n} \frac{e^2}{|R_n + a|} \left[\operatorname{erfc}\left(\frac{|R_n + a|}{2\sqrt{\beta}} \right) - \operatorname{erfc}\left(\frac{|R_n + a|}{2\sqrt{\alpha}} \right) \right] + \frac{4\pi e^2}{\Omega} (\alpha - \beta) + \frac{4\pi e^2}{\Omega} \sum_{K_n \neq 0} \frac{e^{-\beta K_n^2}}{K_n^2} e^{iK_n \cdot a}. \tag{A3.7}$$

Putting $a = 0$ the term in (A3.7) corresponding with $R_n = 0$ appears to be:

$$\lim_{x \to 0} \frac{e^2}{2N} \left(\frac{[\operatorname{erfc}(x/2\sqrt{\beta}) - \operatorname{erfc}(x/2\sqrt{\alpha})]}{x} \right) = \frac{e^2}{2N} \left(\frac{1}{\sqrt{\pi\alpha}} - \frac{1}{\sqrt{\pi\beta}} \right). \tag{A3.8}$$

Appendix 4

According to Carr [5] the two-particle exchange gives the following contribution to the energy of a ferromagnetic lattice:

$$\Delta E_{\mathrm{HF}}^{\mathrm{f}} = -\tfrac{1}{2}\sum_{i\neq j} J_{ij} \tag{A4.1}$$

where J_{ij} is the two-particle exchange integral

$$\begin{aligned} J_{ij} = {} & \int \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) H(1,2) f_0(\boldsymbol{r}_1 - \boldsymbol{R}_j) f_0(\boldsymbol{r}_2 - \boldsymbol{R}_i) \\ & - S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 \int \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) \\ & \times H(1,2) f_0(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0(\boldsymbol{r}_2 - \boldsymbol{R}_j). \end{aligned} \tag{A4.2}$$

The appearing wavefunction f_0 and the overlap S are given by expressions (3.16) and (3.22), respectively, and the effective two-particle Hamiltonian $H(1,2)$ reads

$$\begin{aligned} H(1,2) = {} & \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2N}{\Omega} e^2 \int \mathrm{d}^3 r \left[\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} + \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|} \right] \\ & + e^2 \sum_{m \neq i,j} \int \mathrm{d}^3 r f_0(\boldsymbol{r} - \boldsymbol{R}_m)^2 \left[\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} + \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|} \right]. \end{aligned} \tag{A4.3}$$

In order to compare Carr's calculation of the two-particle exchange energy with the present one (A4.3) is substituted into (A4.2) resulting into

$$\begin{aligned} J_{ij} = {} & \mathrm{e}^{-R_{ij}^2/4\alpha} \left\{ \frac{-\hbar^2 R_{ij}^2}{16 m \alpha^2} + \frac{e^2}{\sqrt{\pi\alpha}} - \frac{e^2}{R_{ij}} \operatorname{erf}\left(\frac{R_{ij}}{2\sqrt{\alpha}} \right) \right. \\ & \left. + 2e^2 \sum_{\boldsymbol{R}_m \neq \boldsymbol{R}_{ij}, 0} \left[\frac{\operatorname{erf}(|\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_{ij}|/2\sqrt{\alpha})}{|\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_{ij}|} - \frac{\operatorname{erf}(R_m/2\sqrt{\alpha})}{R_m} \right] \right\} + \Delta J_{ij} \end{aligned} \tag{A4.4}$$

where $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$ and ΔJ_{ij} is the contribution due to the interaction of the electrons with the positive background,

$$\begin{aligned} \Delta J_{ij} = {} & \int \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) \Delta H(1,2) f_0(\boldsymbol{r}_1 - \boldsymbol{R}_j) f_0(\boldsymbol{r}_2 - \boldsymbol{R}_i) \\ & - S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 \int \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) \\ & \times \Delta H(1,2) f_0(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0(\boldsymbol{r}_2 - \boldsymbol{R}_j) \end{aligned} \tag{A4.5}$$

with

$$\Delta H(1,2) = \frac{-2N}{\Omega} e^2 \int \mathrm{d}^3 r \left[\left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} - \frac{1}{r} \right) + \left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|} - \frac{1}{r} \right) \right]. \tag{A4.6}$$

Now the magnitude of ΔJ_{ij} appears to depend on the way the integration in (A4.6) is performed. Carr's procedure consisted of first integrating over a sphere with a given radius L and afterwards taking the limit $L \to \infty$ giving

$$\Delta H(1,2) = \frac{4\pi N e^2}{3\Omega}(r_1^2 + r_2^2)$$

and

$$\Delta J_{ij} = \frac{-2\pi N e^2}{3\Omega} R_{ij}^2 \mathrm{e}^{-R_{ij}^2/4\alpha}.$$

This actually means that Carr's definition of the jellium model differs from the usual one as given in section 2. According to the usual definition the Coulomb potential $1/r$ must be replaced by the Yukawa potential $\mathrm{e}^{-\mu r}/r$ and the limit $\mu \to 0$ taken after performing the integration. Such a procedure results into $\Delta H(1,2) = \Delta J_{ij} = 0$. Only then the substitution of (A4.4) into (A4.1) leads to the expression (3.28) for the ferromagnetic two-particle exchange energy. That follows directly from the choice $\beta \to \infty$, where β denotes the Ewald parameter. Thus the discrepancy between Carr's and our expression for the exchange energy can be completely understood in terms of two slightly different definitions of the jellium model. This difference in definition, however, does not account for the large discrepancy in critical density for ferromagnetic behaviour. The two critical densities are given by $r_s \simeq 270$ and $r_s \simeq 14$ respectively. Carr's result $r_s \simeq 270$ is based upon the following three approximations for J_{ij}.

(i) The error functions were set equal to one, i.e. J_{ij} was expressed as

$$J_{ij} \simeq \mathrm{e}^{-R_{ij}^2/4\alpha}\left\{ - R_{ij}^2\left[\frac{\hbar^2}{16m\alpha^2} + \frac{2\pi N e^2}{3\Omega}\right] - \frac{3e^2}{R_{ij}} + \frac{e^2}{\sqrt{\pi\alpha}} + 2e^2 \sum_{\boldsymbol{R}_m \neq 0}\left[|\boldsymbol{R}_m - \tfrac{1}{2}\boldsymbol{R}_{ij}|^{-1} - R_m^{-1}\right]\right\}. \tag{A4.7}$$

(ii) The parameter α was given by the Wigner value $\frac{1}{2}r_s^{3/2}a_0^2$.

(iii) The contribution of the sum over $\boldsymbol{R}_m$ was neglected in (A4.7).

These approximations lead to a positive nearest neighbour exchange integral, i.e. to a ferromagnetic lattice, for $r_s \simeq 270$. The approximations (i) and (ii) are both justified because they neglect only irrelevant terms, i.e. terms of order $S(\boldsymbol{R}_{ij})^n$, $n \geqslant 4$. Approximation (iii), however, is certainly not justified as follows directly from a calculation of the first few terms in the sum over $\boldsymbol{R}_m$. This is the main reason for the discrepancy between Carr's and the present result. The correct contribution of the sum over $\boldsymbol{R}_m$ can be found using the Ewald summation method, as done in section 3.

Appendix 5

The interaction operator V is calculated by substituting (4.37) into (4.30). Then we get up to order q^4:

$$\int \mathrm{d}^3k \hat{f}_j(\boldsymbol{k}) \hat{f}_t^*(\boldsymbol{k} \pm \boldsymbol{q})$$

$$
\begin{aligned}
&= \mathrm{e}^{-\alpha q^2/2} \prod_{\hat{\xi}} \{\delta_{\jmath\cdot\hat{\xi},\ell\cdot\hat{\xi}} \pm \mathrm{i}\sqrt{\alpha} q\cdot\hat{\xi}[\sqrt{(\jmath\cdot\hat{\xi}+1)}\,\delta_{\jmath\cdot\hat{\xi}+1,\ell\cdot\hat{\xi}} \\
&\quad + \sqrt{(\ell\cdot\hat{\xi}+1)}\,\delta_{\ell\cdot\hat{\xi}+1,\jmath\cdot\hat{\xi}}] \\
&\quad - \alpha(q\cdot\hat{\xi})^2[\jmath\cdot\hat{\xi}\,\delta_{\jmath\cdot\hat{\xi},\ell\cdot\hat{\xi}} + \tfrac{1}{2}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)}\,\delta_{\jmath\cdot\hat{\xi}+2,\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{2}\sqrt{(\ell\cdot\hat{\xi}+1)(\ell\cdot\hat{\xi}+2)}\,\delta_{\ell\cdot\hat{\xi}+2,\jmath\cdot\hat{\xi}}] \\
&\quad \mp \mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^3[\tfrac{1}{2}(\jmath\cdot\hat{\xi})\sqrt{(\jmath\cdot\hat{\xi}+1)}\,\delta_{\jmath\cdot\hat{\xi}+1,\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{2}(\ell\cdot\hat{\xi})\sqrt{(\ell\cdot\hat{\xi}+1)}\,\delta_{\ell\cdot\hat{\xi}+1,\jmath\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{6}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)(\jmath\cdot\hat{\xi}+3)}\,\delta_{\jmath\cdot\hat{\xi}+3,\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{6}\sqrt{(\ell\cdot\hat{\xi}+1)(\ell\cdot\hat{\xi}+2)(\ell\cdot\hat{\xi}+3)}\,\delta_{\ell\cdot\hat{\xi}+3,\jmath\cdot\hat{\xi}}] \\
&\quad + \alpha^2(q\cdot\hat{\xi})^4[\tfrac{1}{6}(\jmath\cdot\hat{\xi})\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)}\,\delta_{\jmath\cdot\hat{\xi}+2,\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{6}(\ell\cdot\hat{\xi})\sqrt{(\ell\cdot\hat{\xi}+1)(\ell\cdot\hat{\xi}+2)}\,\delta_{\ell\cdot\hat{\xi}+2,\jmath\cdot\hat{\xi}} + \tfrac{1}{4}(\jmath\cdot\hat{\xi})(\jmath\cdot\hat{\xi}-1)\delta_{\jmath\cdot\hat{\xi},\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{24}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)(\jmath\cdot\hat{\xi}+3)(\jmath\cdot\hat{\xi}+4)}\,\delta_{\jmath\cdot\hat{\xi}+4,\ell\cdot\hat{\xi}} \\
&\quad + \tfrac{1}{24}\sqrt{(\ell\cdot\hat{\xi}+1)(\ell\cdot\hat{\xi}+2)(\ell\cdot\hat{\xi}+3)(\ell\cdot\hat{\xi}+4)}\,\delta_{\ell\cdot\hat{\xi}+4,\jmath\cdot\hat{\xi}}] \qquad \text{(A5.1)}
\end{aligned}
$$

and

$$
\begin{aligned}
&\sum_{\jmath,\ell}\int \mathrm{d}^3k\,\hat{f}_\jmath(k)\hat{f}^*_\ell(k\pm q)D^n_{\jmath\ell} = \\
&\qquad \mathrm{e}^{-\frac{1}{2}\alpha q^2}\{S^n_0 + \sum_{\hat{\xi}}[\pm\mathrm{i}\sqrt{\alpha}(q\cdot\hat{\xi})S^n_{\hat{\xi}} - \alpha(q\cdot\hat{\xi})^2 S^n_{2\hat{\xi}} \\
&\qquad + \mp\mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^3 S^n_{3\hat{\xi}} + \alpha^2(q\cdot\hat{\xi})^4 S^n_{4\hat{\xi}}] \\
&\qquad + \sum_{\hat{\xi}\neq\hat{\eta}}[-\tfrac{1}{2}\alpha(q\cdot\hat{\xi})(q\cdot\hat{\eta})S^n_{\hat{\xi}+\hat{\eta}} \mp \mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^2(q\cdot\hat{\eta})S^n_{2\hat{\xi}+\hat{\eta}} \\
&\qquad + \tfrac{1}{2}\alpha^2(q\cdot\hat{\xi})^2(q\cdot\hat{\eta})^2 S^n_{2\hat{\xi}+2\hat{\eta}} + \alpha^2(q\cdot\hat{\xi})^3(q\cdot\hat{\eta})S^n_{3\hat{\xi}+\hat{\eta}}] \\
&\qquad + \sum_{\hat{\zeta}\neq\hat{\xi}\neq\hat{\eta}\neq\hat{\zeta}}[\mp\tfrac{1}{6}\mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})(q\cdot\hat{\eta})(q\cdot\zeta)S^n_{\hat{\xi}+\hat{\eta}+\hat{\zeta}} \\
&\qquad + \tfrac{1}{2}\alpha^2(q\cdot\hat{\xi})^2(q\cdot\hat{\eta})(q\cdot\hat{\zeta})S^n_{2\hat{\xi}+\hat{\eta}+\hat{\zeta}}]\} \qquad \text{(A5.2)}
\end{aligned}
$$

with

$$S^n_0 = \sum_\jmath D^n_{\jmath\jmath}$$

$$S^n_{\hat{\xi}} = \sum_\jmath \sqrt{(\jmath\cdot\hat{\xi}+1)}\,[D^n_{\jmath,\jmath+\hat{\xi}} + D^n_{\jmath+\hat{\xi},\jmath}]$$

$$S^n_{2\hat{\xi}} = \sum_{\mathfrak{z}} [(\mathfrak{z}\cdot\hat{\xi})D^n_{\mathfrak{z}\mathfrak{z}} + \tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}[D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi},\mathfrak{z}}]]$$

$$S^n_{3\hat{\xi}} = \sum_{\mathfrak{z}} [\tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\xi}} + D^n_{\mathfrak{z}+\hat{\xi},\mathfrak{z}}] + \tfrac{1}{6}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)(\mathfrak{z}\cdot\hat{\xi}+3)}[D^n_{\mathfrak{z},\mathfrak{z}+3\hat{\xi}} + D^n_{\mathfrak{z}+3\hat{\xi},\mathfrak{z}}]]$$

$$S^n_{4\hat{\xi}} = \sum_{\mathfrak{z}} [\tfrac{1}{4}\mathfrak{z}\cdot\hat{\xi}(\mathfrak{z}\cdot\hat{\xi}-1)D^n_{\mathfrak{z}\mathfrak{z}} + \tfrac{1}{6}(\mathfrak{z}\cdot\hat{\xi})\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}[D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi},\mathfrak{z}}] + \tfrac{1}{24}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)(\mathfrak{z}\cdot\hat{\xi}+3)(\mathfrak{z}\cdot\hat{\xi}+4)}[D^n_{\mathfrak{z},\mathfrak{z}+4\hat{\xi}} + D^n_{\mathfrak{z}+4\hat{\xi},\mathfrak{z}}]]$$

$$S^n_{\hat{\xi}+\hat{\eta}} = \sum_{\mathfrak{z}} \sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\eta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+\eta,\mathfrak{z}+\hat{\xi}} + D^n_{\mathfrak{z}+\hat{\xi},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\xi}+\hat{\eta},\mathfrak{z}}]$$

$$S^n_{2\hat{\xi}+\hat{\eta}} = \sum_{\mathfrak{z}} [\mathfrak{z}\cdot\hat{\xi}\sqrt{(\mathfrak{z}\cdot\hat{\eta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\eta}} + D_{\mathfrak{z}+\hat{\eta},\mathfrak{z}}] + \tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}[D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\eta},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+2\hat{\xi}+\hat{\eta},\mathfrak{z}}]]$$

$$S^n_{2\hat{\xi}+2\hat{\eta}} = \sum_{\mathfrak{z}} [(\mathfrak{z}\cdot\hat{\xi})(\mathfrak{z}\cdot\hat{\eta})D^n_{\mathfrak{z}\mathfrak{z}} + \tfrac{1}{2}\mathfrak{z}\cdot\hat{\xi}\sqrt{(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\eta}+2)}[D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\eta}} + D^n_{\mathfrak{z}+2\hat{\eta},\mathfrak{z}}] + \tfrac{1}{2}\mathfrak{z}\cdot\hat{\eta}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)}[D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi},\mathfrak{z}}] + \tfrac{1}{4}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\eta}+2)} \times [D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\eta}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\eta},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi},\mathfrak{z}+2\hat{\eta}} + D^n_{\mathfrak{z}+2\hat{\eta}+2\hat{\xi},\mathfrak{z}}]]$$

$$S^n_{3\hat{\xi}+\hat{\eta}} = \sum_{\mathfrak{z}} [\tfrac{1}{2}\mathfrak{z}\cdot\hat{\xi}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\eta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\xi},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\eta},\mathfrak{z}+\hat{\xi}} + D^n_{\mathfrak{z}+\hat{\xi}+\hat{\eta},\mathfrak{z}}] + \tfrac{1}{6}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)(\mathfrak{z}\cdot\hat{\xi}+3)(\mathfrak{z}\cdot\hat{\eta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+3\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\eta},\mathfrak{z}+3\hat{\xi}} + D^n_{\mathfrak{z}+3\hat{\xi},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+3\hat{\xi}+\hat{\eta},\mathfrak{z}}]]$$

$$S^n_{\hat{\xi}+\hat{\eta}+\hat{\zeta}} = \sum_{\mathfrak{z}} \sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\zeta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\xi}+\hat{\eta}+\hat{\zeta}} + D^n_{\mathfrak{z}+\zeta,\mathfrak{z}+\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\xi}+\hat{\eta},\mathfrak{z}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\xi}+\hat{\eta}+\hat{\zeta},\mathfrak{z}} + D^n_{\mathfrak{z}+\eta,\mathfrak{z}+\hat{\xi}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\xi}+\hat{\zeta},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\xi},\mathfrak{z}+\hat{\eta}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\eta}+\hat{\zeta},\mathfrak{z}+\hat{\xi}}]$$

$$S^n_{2\hat{\xi}+\hat{\eta}+\hat{\zeta}} = \sum_{\mathfrak{z}} [\mathfrak{z}\cdot\hat{\xi}\sqrt{(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\zeta}+1)}[D^n_{\mathfrak{z},\mathfrak{z}+\hat{\eta}+\hat{\zeta}} + D^n_{\mathfrak{z}+\eta,\mathfrak{z}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\zeta},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+\hat{\eta}+\hat{\zeta},\mathfrak{z}}] + \tfrac{1}{2}\sqrt{(\mathfrak{z}\cdot\hat{\xi}+1)(\mathfrak{z}\cdot\hat{\xi}+2)(\mathfrak{z}\cdot\hat{\eta}+1)(\mathfrak{z}\cdot\hat{\zeta}+1)} \times [D^n_{\mathfrak{z},\mathfrak{z}+2\hat{\xi}+\hat{\eta}+\hat{\zeta}} + D^n_{\mathfrak{z}+\zeta,\mathfrak{z}+2\hat{\xi}+\hat{\eta}} + D^n_{\mathfrak{z}+2\hat{\xi}+\mathfrak{z}+\hat{\eta}+\hat{\zeta}} + D^n_{\mathfrak{z}+2\hat{\xi}+\hat{\zeta},\mathfrak{z}+\hat{\eta}} + D^n_{\mathfrak{z}+\eta,\mathfrak{z}+2\hat{\xi}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\eta}+\hat{\zeta},\mathfrak{z}+2\hat{\xi}} + D^n_{\mathfrak{z}+2\hat{\xi}+\hat{\eta},\mathfrak{z}+\hat{\zeta}} + D^n_{\mathfrak{z}+\hat{\eta}+2\hat{\xi}+\hat{\zeta},\mathfrak{z}}]]. \tag{A5.3}$$

Using the effective properties (4.34) and (4.35) of the operators $D^n_{j_1 j_2}$ the following expressions for the operators as defined in (A5.3) are obtained:

$$
\begin{aligned}
&S^n_{\mathbf{0}} = 1 \qquad S^n_{2\hat{\xi}} = \tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{2} \\
&S^n_{3\hat{\xi}} = \tfrac{1}{6} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{2} S^n_{\hat{\xi}} \\
&S^n_{4\hat{\xi}} = \tfrac{1}{24} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} + \tfrac{1}{8} \\
&S^n_{\hat{\xi}+\hat{\eta}} = S^n_{\hat{\xi}} S^n_{\hat{\eta}}, S^n_{2\hat{\xi}+\hat{\eta}} = \tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} - \tfrac{1}{2} S^n_{\hat{\eta}} \\
&S^n_{2\hat{\xi}+2\hat{\eta}} = \tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\eta}} - \tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{4} S^n_{\hat{\eta}} S^n_{\hat{\eta}} + \tfrac{1}{4} \\
&S^n_{3\hat{\xi}+\hat{\eta}} = \tfrac{1}{6} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} - \tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\eta}} \\
&S^n_{\hat{\xi}+\hat{\eta}+\hat{\zeta}} = S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\zeta}}, S^n_{2\hat{\xi}+\hat{\eta}+\hat{\zeta}} = \tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\zeta}} - \tfrac{1}{2} S^n_{\hat{\eta}} S^n_{\hat{\zeta}}.
\end{aligned}
\tag{A5.4}
$$

Substituting (A5.4) into (A5.2) we arrive at:

$$
\begin{aligned}
&\sum_{j,\ell} \int \mathrm{d}^3 k \hat{f}_j(k) \hat{f}^*_\ell(k \pm q) D^n_{j\ell} \\
&\quad = \mathrm{e}^{-\frac{1}{2}\alpha q^2} \{1 + \sum_{\hat{\xi}} [\pm \mathrm{i}\sqrt{\alpha}(q\cdot\hat{\xi}) S^n_{\hat{\xi}} - \alpha(q\cdot\hat{\xi})^2 [\tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{2}] \\
&\qquad + \mp \mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^3 [\tfrac{1}{6} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{2} S^n_{\hat{\xi}}] \\
&\qquad + \alpha^2 (q\cdot\hat{\xi})^4 [\tfrac{1}{24} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} + \tfrac{1}{8}]] \\
&\qquad + \sum_{\hat{\xi}\neq\hat{\eta}} [-\tfrac{1}{2}\alpha(q\cdot\hat{\xi})(q\cdot\hat{\eta}) [S^n_{\hat{\xi}} S^n_{\hat{\eta}}] \mp \mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^2 (q\cdot\hat{\eta}) [\tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} - \tfrac{1}{2} S^n_{\hat{\eta}}] \\
&\qquad + \tfrac{1}{2}\alpha^2 (q\cdot\hat{\xi})^2 (q\cdot\hat{\eta})^2 [\tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\eta}} - \tfrac{1}{4} S^n_{\hat{\xi}} S^n_{\hat{\xi}} - \tfrac{1}{4} S^n_{\hat{\eta}} S^n_{\hat{\eta}} + \tfrac{1}{4}] \\
&\qquad + \alpha^2 (q\cdot\hat{\xi})^3 (q\cdot\hat{\eta}) [\tfrac{1}{6} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} - \tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\eta}}]] \\
&\qquad + \sum_{\hat{\zeta}\neq\hat{\xi}\neq\hat{\eta}\neq\hat{\zeta}} [\mp \tfrac{1}{6}\mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})(q\cdot\hat{\eta})(q\cdot\hat{\zeta}) S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\zeta}} \\
&\qquad + \tfrac{1}{2}\alpha^2 (q\cdot\hat{\xi})^2 (q\cdot\hat{\eta})(q\cdot\hat{\zeta}) [\tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\eta}} S^n_{\hat{\zeta}} - \tfrac{1}{2} S^n_{\hat{\eta}} S^n_{\hat{\zeta}}]]\}.
\end{aligned}
\tag{A5.5}
$$

Now the interaction operator V is given by

$$
\begin{aligned}
V \equiv &\sum_{j_1 j_2 \ell_1 \ell_2} \tfrac{1}{2} \sum_{n\neq m} \mathrm{e}^{\mathrm{i}q\cdot R_{nm}} \frac{4\pi e^2}{\Omega q^2} \\
&\times \int \mathrm{d}^3 k \mathrm{d}^3 k' \hat{f}_{j_1}(k) \hat{f}_{j_2}(k') \hat{f}^*_{\ell_2}(k'+q) \hat{f}^*_{\ell_1}(k-q) D^n_{j_1\ell_1} D^m_{j_2\ell_2} \\
= &\tfrac{1}{2} \sum_{n\neq m} \mathrm{e}^{\mathrm{i}q\cdot R_{nm}} \frac{4\pi e^2}{\Omega q^2} \mathrm{e}^{-\alpha q^2} \{1 + \sum_{\hat{\xi}} [-\mathrm{i}\sqrt{\alpha}(q\cdot\hat{\xi}) [S^n_{\hat{\xi}} - S^m_{\hat{\xi}}] \\
&- \alpha(q\cdot\hat{\xi})^2 [\tfrac{1}{2} S^n_{\hat{\xi}} S^n_{\hat{\xi}} + \tfrac{1}{2} S^m_{\hat{\xi}} S^m_{\hat{\xi}} - 1 - S^n_{\hat{\xi}} S^m_{\hat{\xi}}] + \mathrm{i}\alpha\sqrt{\alpha}(q\cdot\hat{\xi})^3 [\tfrac{1}{6} S^n_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}} \\
&- S^n_{\hat{\xi}} - \tfrac{1}{6} S^m_{\hat{\xi}} S^m_{\hat{\xi}} S^m_{\hat{\xi}} + S^m_{\hat{\xi}} + \tfrac{1}{2} S^n_{\hat{\xi}} S^m_{\hat{\xi}} S^m_{\hat{\xi}} - \tfrac{1}{2} S^m_{\hat{\xi}} S^n_{\hat{\xi}} S^n_{\hat{\xi}}]
\end{aligned}
$$

$$
\begin{aligned}
&+\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^4\big[\tfrac{1}{24}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}\\
&+\tfrac{1}{24}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}-\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\xi}-\tfrac{1}{2}S^m_{\hat\xi}S^m_{\hat\xi}+\tfrac{1}{2}\\
&+\tfrac{1}{4}S^n_{\hat\xi}S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}-\tfrac{1}{6}S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}+S^n_{\hat\xi}S^m_{\hat\xi}-\tfrac{1}{6}S^m_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}\big]\big]\\
&+\sum_{\hat\xi\neq\hat\eta}\big[-\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\big[\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{2}S^m_{\hat\xi}S^m_{\hat\eta}-S^n_{\hat\xi}S^m_{\hat\eta}\big]\\
&+\mathrm{i}\alpha\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\big[\tfrac{1}{2}S^n_{\hat\eta}S^m_{\hat\xi}S^m_{\hat\xi}-S^n_{\hat\eta}-\tfrac{1}{2}S^m_{\hat\eta}S^n_{\hat\xi}S^n_{\hat\xi}+S^m_{\hat\eta}+\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}\\
&-\tfrac{1}{2}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}+S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}-S^m_{\hat\xi}S^n_{\hat\xi}+S^n_{\hat\eta}\big]\\
&+\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})^2\big[\tfrac{1}{4}S^n_{\hat\xi}S^n_{\hat\xi}S^m_{\hat\eta}S^m_{\hat\eta}-\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\xi}-\tfrac{1}{2}S^m_{\hat\eta}S^m_{\hat\eta}+\tfrac{1}{2}\\
&-\tfrac{1}{2}S^n_{\hat\eta}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}+S^n_{\hat\eta}S^m_{\hat\eta}-\tfrac{1}{2}S^m_{\hat\eta}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\eta}S^m_{\hat\xi}S^m_{\hat\eta}\\
&+\tfrac{1}{8}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}S^n_{\hat\eta}+\tfrac{1}{8}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}S^m_{\hat\eta}\big]+\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\big[-\tfrac{1}{6}S^n_{\hat\eta}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}\\
&+\tfrac{1}{2}S^n_{\hat\eta}S^m_{\hat\xi}-\tfrac{1}{6}S^m_{\hat\eta}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}+\tfrac{1}{2}S^m_{\hat\eta}S^n_{\hat\xi}-\tfrac{1}{2}S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}+\tfrac{1}{2}S^m_{\hat\xi}S^m_{\hat\eta}\\
&-\tfrac{1}{2}S^m_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{2}S^m_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{2}S^n_{\hat\xi}S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}-S^m_{\hat\xi}S^m_{\hat\eta}\\
&+\tfrac{1}{2}S^m_{\hat\xi}S^m_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}-S^n_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{6}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}+\tfrac{1}{6}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}\big]\big]\\
&+\sum_{\hat\zeta\neq\hat\xi\neq\hat\eta\neq\hat\zeta}\big[\mathrm{i}\alpha^2\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\zeta}})\times\big[\tfrac{1}{2}S^n_{\hat\zeta}S^m_{\hat\xi}S^m_{\hat\eta}-\tfrac{1}{2}S^m_{\hat\zeta}S^n_{\hat\xi}S^n_{\hat\eta}\\
&+\tfrac{1}{6}S^n_{\hat\xi}S^n_{\hat\eta}S^n_{\hat\zeta}-\tfrac{1}{6}S^m_{\hat\xi}S^m_{\hat\eta}S^m_{\hat\zeta}\big]+\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\zeta}})\big[\tfrac{1}{4}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}S^n_{\hat\zeta}\\
&+\tfrac{1}{4}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}S^m_{\hat\zeta}\\
&-\tfrac{1}{2}S^n_{\hat\eta}S^n_{\hat\zeta}-\tfrac{1}{2}S^m_{\hat\eta}S^m_{\hat\zeta}-\tfrac{1}{2}S^n_{\hat\zeta}S^m_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}+S^n_{\hat\zeta}S^m_{\hat\eta}\\
&-\tfrac{1}{2}S^m_{\hat\zeta}S^n_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}-\tfrac{1}{2}S^n_{\hat\xi}S^m_{\hat\xi}S^m_{\hat\eta}S^m_{\hat\zeta}-\tfrac{1}{2}S^m_{\hat\xi}S^n_{\hat\xi}S^n_{\hat\eta}S^n_{\hat\zeta}\\
&+\tfrac{1}{4}S^n_{\hat\xi}S^n_{\hat\xi}S^m_{\hat\zeta}S^m_{\hat\eta}+\tfrac{1}{4}S^m_{\hat\xi}S^m_{\hat\xi}S^n_{\hat\zeta}S^n_{\hat\eta}+S^n_{\hat\xi}S^n_{\hat\eta}S^m_{\hat\xi}S^m_{\hat\zeta}\big]\big]\big\}
\end{aligned}
\tag{A5.6}
$$

where all terms containing q^M, $M > 4$, have been neglected. In terms of the operators $\boldsymbol{S}_n$, given by (4.39), we can express the interaction operator up to order q^4 as

$$
\begin{aligned}
V=\tfrac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}'\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}\big\{1+\sqrt{\alpha}\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n)\big]\\
+\tfrac{1}{2}\alpha\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n)\big]^2+\tfrac{1}{6}\alpha\sqrt{\alpha}\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n)\big]^3+\tfrac{1}{24}\alpha^2\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n)\big]^4\\
+\alpha q^2+\alpha\sqrt{\alpha}\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n\big]q^2+\tfrac{1}{2}\alpha^2\big[q^2+\big[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{S}_m-\boldsymbol{S}_n)\big]^2\big]q^2\big\}
\end{aligned}
\tag{A5.7}
$$

with

$$
\tfrac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}'\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega q^2}\mathrm{e}^{-\alpha q^2}=E_{\mathrm{CI}}+2N\left[\frac{4\pi Ne^2\alpha}{\Omega}-\tfrac{1}{2}e^2\sum_{n\neq 0}\frac{1}{R_n}\operatorname{erfc}\left(\frac{R_n}{2\sqrt{\alpha}}\right)\right]
$$

$$
\tfrac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}'\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega}\mathrm{e}^{-\alpha q^2}=2N\left[\frac{-4\pi Ne^2}{\Omega}+\sum_{n\neq 0}\frac{e^2}{4\alpha\sqrt{\pi\alpha}}\mathrm{e}^{-R_n^2/4\alpha}\right]
$$

$$\tfrac{1}{2}\sum_{n\neq m}\sum_{q}{}' e^{iq\cdot R_{nm}}\frac{4\pi e^2}{\Omega}q^2 e^{-\alpha q^2} = 2N\sum_{n\neq 0}\frac{e^2}{16\alpha^3\sqrt{\pi\alpha}}(6\alpha - R_n^2)e^{-R_n^2/4\alpha}$$

$$\tfrac{1}{2}\sum_{n\neq m}\sum_{q}{}' e^{iq\cdot R_{nm}}\frac{4\pi e^2}{\Omega}[q\cdot(S_n - S_m)]^2 e^{-\alpha q^2}$$

$$= 2N\sum_{n\neq 0}\frac{e^2}{16\alpha^3\sqrt{\pi\alpha}}(5|S_n - S_m|^2\alpha - \tfrac{1}{2}R_n^2|S_n - S_m|^2$$

$$- [R_n\cdot(S_n - S_m)]^2)e^{-R_n^2/4\alpha} \tag{A5.8}$$

and

$$\tfrac{1}{2}\sum_{n\neq m}\sum_{q}{}' e^{iq\cdot R_{nm}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}\begin{cases}[\sqrt{\alpha}iq\cdot(S_m - S_n)] & = 0\\ \alpha\sqrt{\alpha}[iq\cdot(S_m - S_n)]q^2 & = 0\end{cases} \tag{A5.9}$$

where use is made of the cubic symmetry of the lattice in calculating (A5.9). Substitution of (A5.8) and (A5.9) into (A5.7) leads to expression (4.38), where we have neglected all terms containing $\exp[-R_n^2/4\alpha]$ and $\operatorname{erfc}(R_n/2\sqrt{\alpha})$.

Higher order contibutions to V, i.e. contributions containing $(S_m - S_n)^M$, $M > 4$, can be found analogously and are expected to be given by the following expression, that holds also for $M = 3$ and $M = 4$:

$$V_M = \tfrac{1}{2}\sum_{n\neq m}\sum_{q}{}' e^{iq\cdot R_{nm}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}\left[\frac{1}{M!}\alpha^{M/2}[iq\cdot(S_m - S_n)]^M\right]$$

$$= \tfrac{1}{2}\sum_{n\neq m}\left[\frac{1}{M!}\alpha^{M/2}[(S_m - S_n)\cdot\nabla_{nm}]^M\right]\left(\frac{e^2}{R_{nm}}\right) \tag{A5.10}$$

where all terms of the order of the overlap are neglected, and the gradient operator ∇_{nm} is given by

$$\nabla_{nm} = \sum_{\hat{\xi}}\hat{\xi}\frac{\partial}{\partial(R_{nm}\cdot\hat{\xi})}. \tag{A5.11}$$

Using the results of section 4 the effective Hamiltonian can be written as

$$H_{\text{eff}} = E_{\text{Cl}} + \sum_{k\lambda}(\tfrac{1}{2} + A_{k\lambda}^{+}A_{k\lambda})\hbar\omega_{k\lambda} + \sum_{M=3}^{\infty}V_M \tag{A5.12}$$

where the boson operators $A_{k\lambda}^{(+)}$ are related with the operators S_n according to

$$S_n = \frac{1}{\sqrt{2N}}\sum_{k\lambda}\sqrt{\frac{\hbar}{2m\alpha\omega_{k\lambda}}}e^{ik\cdot R_n}\varepsilon_{k\lambda}[A_{k\lambda}^{+} + A_{k\lambda}]. \tag{A5.13}$$

Substituting (A5.13) into (A5.10) we find that the contribution of V_M to the effective Hamiltonian consists of terms proportional to $R_{mn}^{-M-1}\omega_{k\lambda}^{-\frac{1}{2}M}$. This implies that V_M is proportional to $r_s^{-\frac{1}{4}M-1}$ as R_{mn} and $\omega_{k\lambda}$ are proportional to r_s and $r_s^{-3/2}$, respectively, and V_M is independent of α. On the basis of perturbation theory we can then conclude that the ground state energy of (A5.12) is a power series in $r_s^{-1/4}$ with the additional property that all odd powers of $r_s^{-1/4}$ do not appear.

Appendix 6

The ground state of the low density electron system can be expressed as (cf (4.13))

$$|\psi_0\rangle = \sum_{\substack{j_1,\ldots,j_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_{2N}}(0) d^+_{j_1\sigma_1}(\boldsymbol{R}_1),\ldots,d^+_{j_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle. \tag{A6.1}$$

Up to order $r_s^{-3/2}$ the coefficients $A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_{2N}}(0)$ are determined by the requirement

$$A_{k\lambda}|\psi_0\rangle = 0 \tag{A6.2}$$

for all k and λ. The operators $A_{k\lambda}$ are given by, according to (4.31), (4.40), (4.47), (4.51) and (4.54),

$$A_{k\lambda} = \frac{1}{\sqrt{2N}} \sum_{i,\hat{\xi},j,\sigma} \left[\alpha^{k\lambda}_{i\hat{\xi}} d^+_{j+\hat{\xi}\sigma}(\boldsymbol{R}_i) d_{j\sigma}(\boldsymbol{R}_i) + \beta^{k\lambda}_{i\hat{\xi}} d^+_{j\sigma}(\boldsymbol{R}_i) d_{j+\hat{\xi}\sigma}(\boldsymbol{R}_i)\right] \sqrt{(j\cdot\hat{\xi}+1)} \tag{A6.3}$$

with

$$\begin{aligned} \alpha^{k\lambda}_{i\hat{\xi}} &= \left(\left[\frac{m\omega_{k\lambda}\alpha}{2\hbar}\right]^{1/2} + \left[\frac{\hbar}{8m\omega_{k\lambda}\alpha}\right]^{1/2}\right) e^{ik\cdot R_i} \varepsilon_{k\lambda}\cdot\hat{\xi} \\ \beta^{k\lambda}_{i\hat{\xi}} &= \left(\left[\frac{m\omega_{k\lambda}\alpha}{2\hbar}\right]^{1/2} - \left[\frac{\hbar}{8m\omega_{k\lambda}\alpha}\right]^{1/2}\right) e^{ik\cdot R_i} \varepsilon_{k\lambda}\cdot\hat{\xi}. \end{aligned} \tag{A6.4}$$

Substituting (A6.3) into (A6.2) we obtain

$$\sum_{i,\hat{\xi}} \sum_{\substack{j_1,\ldots,j_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} \left[A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_i-\hat{\xi}\ldots j_{2N}}(0)\sqrt{(j_i\cdot\hat{\xi})}\alpha^{k\lambda}_{i\hat{\xi}} + A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_i+\hat{\xi}\ldots j_{2N}}(0)\sqrt{(j_i\cdot\hat{\xi}+1)}\beta^{k\lambda}_{i\hat{\xi}}\right] \times d^+_{j_1\sigma_1}(\boldsymbol{R}_1),\ldots,d^+_{j_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle = 0 \tag{A6.5}$$

for all k and λ. Thus for all sets $\{j_1,\ldots,j_{2N}\}$ and $\{\sigma_1,\ldots,\sigma_{2N}\}$ we have the following $6N$ linear equations:

$$\sum_{i,\hat{\xi}} \left[\sqrt{(j_i\cdot\hat{\xi})}\alpha^{k\lambda}_{i\hat{\xi}} A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_i-\hat{\xi}\ldots j_{2N}}(0) + \sqrt{(j_i\cdot\hat{\xi}+1)}\beta^{k\lambda}_{i\hat{\xi}} A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_i+\hat{\xi}\ldots j_{2N}}(0)\right] = 0 \tag{A6.6}$$

for all k and λ. These equations give rise to recursion relations between coefficients $A^{\sigma_1\ldots\sigma_{2N}}_{j_1\ldots j_{2N}}(0)$ with different $j = \sum_{i,\hat{\xi}} j_i\cdot\hat{\xi}$ starting with $j = 0$ and $j = 1$. The complexity of these relations increases with increasing j and actually prevents a calculation of all coefficients. Nevertheless a few conclusions can be drawn from (A6.6).

(i) The coefficients with j odd are all zero. This can easily be seen for $j = 1$ by substituting $j_1 = j_2 = \ldots = j_{2N} = 0$ into (A6.6). As the recursion relations only

contain coefficients with $j = j_0$ and $j = j_0 + 2$, $j_0 = 1, 2, 3, \ldots$, all coefficients with j odd must be zero.

(ii) The coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{j_1 \ldots j_{2N}}(0)$ with j even can all be expressed in terms of $A^{\sigma_1 \ldots \sigma_{2N}}_{0 \ldots 0}(0)$. They decrease as $[(j_i \cdot \hat{\xi})!]^{-1/2}$ with increasing $j_i \cdot \hat{\xi}$, $i = 1, \ldots, 2N$. The coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{0 \ldots 0}(0)$ can be chosen almost completely arbitrarily, the only restriction being that the ground state must be normalized. This means that the ground state is degenerate with respect to all possible spin configurations $\{\sigma_1, \ldots, \sigma_{2N}\}$ of the lattice. As discussed in section 3 this is due to the neglect of exchange contributions to the ground state energy.

References

[1] Wigner E 1938 *Trans. Faraday Soc.* **34** 678
[2] Care C M and March M H 1975 *Adv. Phys.* **24** 101
[3] Peierls R E 1955 *Quantum Theory of Solids* (Oxford: Clarendon)
[4] Sholl C A 1967 *Proc. Phys. Soc. London* **92** 434
[5] Carr W J 1961 *Phys. Rev.* **122** 1437
[6] Mahan G D 1981 *Many-Particle Physics* (New York: Plenum)
[7] Born M and Huang K 1954 *Dynamical Theory of Crystal Lattices* (Oxford: Oxford University Press)
[8] Brenig W 1962 *Z. Phys.* **171** 60
[9] Fredkin D R and Werthamer N R 1964 *Phys. Rev.* **138A** 1527
[10] Pietrass B 1967 *Phys. Status Solidi* **24** 571
[11] Carr W J, Coldwell-Horsfall R A and Fein A E 1961 *Phys. Rev.* **124** 747
[12] Kugler A A 1969 *Ann. Phys., NY* **53** 133
[13] Horner W 1967 *Z. Phys.* **205** 72
[14] Fukuyama 1975 *Solid State Commun.* **17** 1323
[15] Fukuyama H 1976 *Surface Science* **58** 320
[16] Fukuyama H and McClure J W 1975 *Solid State Commun.* **17** 1327
[17] Bardeen J, Cooper L N and Schrieffer J R 1957 *Phys. Rev.* **108** 1175
[18] Rickayzen G 1965 *Theory of Superconductivity* (New York: Wiley)
[19] Kubo R 1959 *Lectures in Theoretical Physics* vol I (New York: Wiley)
[20] London F 1961 *Superfluids* vol 1 (New York: Dover) London stressed that a Meissner–Ochsenfeld effect can occur as soon as the system's wavefunction is rigid in the sense that it is hardly affected by a magnetic field.