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General Hartree–Fock Solutions for a One Dimensional δ-Function Gas

Besnik Sykja* and Jean-Louis Calais**

Quantum Chemistry Group, University of Uppsala, Box 518, S-751 20 Uppsala, Sweden

The one dimensional fermion gas with δ-function interactions is studied within the General Hartree–Fock (GHF) framework. Solutions of the eight Fukutome types are constructed by pairing and the corresponding gap equations are solved. The character of the solutions is studied as a function of the particle density.

Key words: General Hartree–Fock equations – Fukutome classes – Gap equation – One dimensional fermion gas – Delta function interaction.

Introduction

Model calculations, even for seemingly unrealistic systems, are often valuable for getting familiar with methods and procedures which have so far not been applied to the cases they have been primarily designed for. The Hartree–Fock method has certainly been applied to numerous systems and its properties are quite well known. That is not the case, however, with what we prefer to call the General Hartree–Fock (GHF) method: a one determinantal scheme without any restrictions whatsoever on the spin orbitals used in the determinant. As a step in that direction we present in this paper a GHF study of a one dimensional Fermi gas with δ-function interactions.

Herrick and Stillinger [1] have noticed that for a two-particle system confined to one dimension the ordinary interaction is equivalent to a δ-function interaction. Although for more than two particles no similar result seems to be known, this indicates a certain correspondence between the problem to be studied in this paper and a three-dimensional electronic system.

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* Permanent address: Physical Chemistry Department, Tirana University, Tirana, Albania.

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The δ-function interaction potential has been used by many authors for one electron atoms [2, 3], two electron atoms [4–7], a collection of a large number of interacting boson-fermion systems [8] and finally for the electron gas in one dimension [9] and three dimensions [10–11]. As discussed elsewhere [12–13], the δ-function potential not only leads to exactly solvable equations which allows a test of various theoretical models, but at the same time exhibits some connections with the real problem, as for instance the fulfilment of the same virial theorem. Some estimates of various properties of the system are possible by choosing the strength of the δ-function potential:

$$V_{ij}=\gamma\delta(x_i-x_j) \tag{1}$$

in a semiempirical manner [14].

We should not forget, of course, the differences as compared with the three-dimensional coulomb problem, the most important one being perhaps the existence in the case of He like ions, of only one bound state. Having that in mind we will be concerned only with the *ground state* of the one dimensional Fermi gas with δ-function interactions and we will try to find the best ground state in the *one determinant approximation.*

Recent studies of chemical reactions [15], linear chains [16], the electron gas [17] within the GHF-framework, have shown, on one hand, that it is too early to abandon the one determinant approximation for molecular systems, where the various GHF-states or the corresponding projected ones, may in many cases compete with CI-methods [18], on the other that such states for extended systems offer sufficient flexibility to account for many correlation effects.

AMO (Alternant Molecular Orbitals) [19] and SDW (Spin Density Waves) [9–10] were early examples for extended systems of the existence of single determinant states of broken symmetry type with lower energy than the conventional, restricted Hartree–Fock (RHF). What we now call AMO's were also used in Slater's theory of antiferromagnetism [20]. After the derivation of general instability equations for a RHF state [33a] a lot of work has been done, especially in cyclic polyenes and linear polymer chains [21–26].

Given a set of N spin orbitals occupied in an RHF-state and $M-N$ virtual spin orbitals forming together the set

$$\begin{aligned}\boldsymbol{\psi}&=\{\psi_1,\psi_2,\dots\psi_N;\psi_{N+1},\dots\psi_M\}\\&=\{\boldsymbol{\psi}_{\text{occ}};\boldsymbol{\psi}_{\text{unocc}}\}\end{aligned} \tag{2a}$$

the most general determinant $|\Phi\rangle$ [27b], can be built up of the first N spin orbitals of the set

$$\begin{aligned}\boldsymbol{\phi}&=\{\phi_1,\phi_2,\dots\phi_N;\phi_{N+1},\dots\phi_M\}\\&=\{\boldsymbol{\phi}_{\text{occ}},\boldsymbol{\phi}_{\text{unocc}}\}\\&=\{\boldsymbol{\psi}_{\text{occ}},\boldsymbol{\psi}_{\text{unocc}}\}\boldsymbol{U}(\boldsymbol{\lambda})\end{aligned} \tag{2b}$$

where

$$U(\boldsymbol{\lambda}) = \begin{pmatrix} \boldsymbol{C}(\boldsymbol{\lambda}) & -\boldsymbol{S}^{+}(\boldsymbol{\lambda}) \\ \boldsymbol{S}(\boldsymbol{\lambda}) & \bar{\boldsymbol{C}}(\boldsymbol{\lambda}) \end{pmatrix} \tag{3}$$

is a unitary matrix. $\boldsymbol{C}(\boldsymbol{\lambda})$ is a hermitian $N \times N$ matrix, $\bar{\boldsymbol{C}}(\boldsymbol{\lambda})$ hermitian $(M-N) \times (M-N)$ matrix, and $\boldsymbol{S}(\boldsymbol{\lambda})$ a $(M-N) \times N$ matrix. The unitarity of $\boldsymbol{U}(\boldsymbol{\lambda})$ implies certain relations between $\boldsymbol{S}(\boldsymbol{\lambda})$, $\boldsymbol{C}(\boldsymbol{\lambda})$ and $\bar{\boldsymbol{C}}(\boldsymbol{\lambda})$.

From (2) we have:

$$\boldsymbol{\phi}_{\text{occ}} = \boldsymbol{\psi}_{\text{occ}} \cdot \boldsymbol{C}(\boldsymbol{\lambda}) + \boldsymbol{\psi}_{\text{unocc}} \cdot \boldsymbol{S}(\boldsymbol{\lambda}) \tag{4}$$

and by assumption, $\boldsymbol{\psi}$ – is a symmetry adapted basis with respect to all symmetry elements present in the system. $\boldsymbol{\lambda}$ is a matrix of variational parameters (λ_{ij}) which could lead to a state $|\Phi\rangle$ having lower energy than $|\Psi\rangle$.

In a general spin orbital basis:

$$\phi_i(\vec{r}, \zeta) = \phi_{i1}(\vec{r})\alpha(\zeta) + \phi_{i2}(\vec{r})\beta(\zeta) \tag{5}$$

the most general symmetry group is $P \times S \times T$ where P is the spatial point group of the system, S the group of spin rotations and T the group of time reversal. The group theoretical analysis leads to a general classification of the GHF-states [(27, 28)]. Thouless [33a] was the first to show the unitary connection between two determinants $|\Phi\rangle$ and $|\Psi\rangle$, but the specification (3) of the unitary transformation of the basis $\boldsymbol{\psi}$ – and especially the (Eq. 4) made possible an investigation of the symmetry connection of two determinants $|\Phi\rangle$ and $|\Psi\rangle$ via the symmetry of the variational parameter matrix λ, which also gave a classification of instabilities.

We have previously studied [29] a simple connection between this general procedure and a "pairing scheme" – where instead of (4) we mix one occupied state with an unoccupied one:

$$\begin{aligned} &\phi_k(\vec{r}, \zeta) = \psi_k(\vec{r}, \zeta)u_k + \psi_{\bar{k}}(\vec{r}, \zeta)v_k \\ &k = 1, 2, \ldots, N \qquad u_k^2 + v_k^2 = 1 \\ &\bar{k} = N+1, N+2, \ldots, M \qquad u_k^2 - v_k^2 = \lambda_k. \end{aligned} \tag{6}$$

The best matrix $\boldsymbol{\lambda}$ or the best coefficients $u_{k'}v_{k'}$ are determined by the variational principle. If a pairing scheme like Eq. (6) is used the minimization can be expressed in terms of a gap equation [31]. In the present paper we use the orbital forms of the gap equation developed by one of the authors [30].

The paper is organized as follows. In Section 2 we present the model system, the structure of the density matrix and gap equations for each of GHF-states. In Section 3 we obtain numerical solutions of the gap equations and discuss the obtained results.

2. GHF-States of the One Dimensional Fermi Gas with δ-Function Interaction

We use z as the space coordinate. A uniform positive background is assumed so as to have a neutral system.

The length of the chain is:

$$L = N \cdot a \tag{7}$$

where $N = 2(2m+1)$ is the number of particles. The "unit cell" length a is a measure of the inverse density:

$$n = \frac{N}{L} = \frac{1}{a}. \tag{8}$$

As is well known, the plane waves:

$$\eta(k, z) = \frac{1}{\sqrt{L}} e^{ikz} \tag{9}$$

with

$$k = \frac{2\pi}{Na}\kappa$$

$$-\frac{\pi}{a} \le k < \frac{\pi}{a}$$

$$-\frac{N}{2} \le \kappa < \frac{N}{2}$$

multiplied by the spin functions $\alpha(\zeta)$ and $\beta(\zeta)$ form a possible set of solutions of the Hartree–Fock equation for the one dimensional electron gas with either Coulomb potentials or δ-potentials.

In the general spin orbital basis Eq. (5), the Fock–Dirac density matrix is:

$$\rho(\vec{r}_1\zeta_1; \vec{r}_1'\zeta_1') = (\alpha \quad \beta)\begin{pmatrix} \sum_{i=1}^{N} |\phi_{i1}\rangle\langle\phi_{i1}| & \sum_{i=1}^{N} |\phi_{i1}\rangle\langle\phi_{i2}| \\ \sum_{i=1}^{N} |\phi_{i2}\rangle\langle\phi_{i1}| & \sum_{i=1}^{N} |\phi_{i2}\rangle\langle\phi_{i2}| \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \tag{10}$$

which can be written as

$$\rho(\vec{r}_1\zeta_1; \vec{r}_1'\zeta_1') = (\alpha \quad \beta)\begin{pmatrix} \rho_{11}(\vec{r}_1; \vec{r}_1') & \rho_{12}(\vec{r}_1; \vec{r}_1') \\ \rho_{21}(\vec{r}_1; \vec{r}_1') & \rho_{22}(\vec{r}_1; \vec{r}_1') \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix}.$$

By introducing:

$$N(\vec{r}_1; \vec{r}_1') = \rho_{11}(\vec{r}_1; \vec{r}_1') + \rho_{22}(\vec{r}_1; \vec{r}_1') \tag{11}$$

$$S_x(\vec{r}_1; \vec{r}_1') = \tfrac{1}{2}[\rho_{12}(\vec{r}_1, \vec{r}_1') + \rho_{21}(\vec{r}_1; \vec{r}_1')] \tag{12a}$$

$$S_y(\vec{r}_1;\vec{r}_1')=\frac{1}{2i}[\rho_{21}(\vec{r}_1;\vec{r}_1')-\rho_{12}(\vec{r}_1;\vec{r}_1')] \tag{12b}$$

$$S_z(\vec{r}_1;\vec{r}_1')=\tfrac{1}{2}[\rho_{11}(\vec{r}_1;\vec{r}_1')-\rho_{22}(\vec{r}_1;\vec{r}_1')] \tag{12c}$$

we get

$$\rho(\vec{r}_1,\zeta_1;\vec{r}_1',\varphi_1')=(\alpha\beta)\boldsymbol{Q}(\vec{r}_1;\vec{r}_1')\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

with

$$\boldsymbol{Q}(\vec{r}_1;\vec{r}_1')=\tfrac{1}{2}N(\vec{r}_1;\vec{r}_1')\cdot\mathbf{1}_2+\vec{\sigma}\cdot\vec{S}(\vec{r}_1,\vec{r}_1'). \tag{13}$$

Here $\vec{\sigma}=\{\sigma_x,\sigma_y,\sigma_z\}$ is the Pauli matrix vector and

$$\begin{aligned}\vec{S}(\vec{r}_1;\vec{r}_1')&=\{S_x(\vec{r}_1;\vec{r}_1'),S_y(\vec{r}_1;\vec{r}_1'),S_z(\vec{r}_1;\vec{r}_1')\}\\ &=\int_{\zeta_1=\zeta_1'}\vec{s}\cdot\rho(\vec{r}_1,\zeta_1;\vec{r}_1',\zeta_1')\,d\zeta_1\end{aligned} \tag{14}$$

where $\vec{s}$ is the spin operator.

The effective one electron hamiltonian becomes:

$$\mathcal{H}_{\text{eff}}(\vec{r}_1)=F(\vec{r}_1)\cdot\mathbf{1}_2+\vec{\sigma}\cdot\vec{G}(\vec{r}_1) \tag{15}$$

where

$$\begin{aligned}F(\vec{r}_1)=h_1&+\int h_{12}N(\vec{r}_2;\vec{r}_2')\,d\vec{r}_2\\ &-\frac{1}{2}\int h_{12}\cdot P_{12}^r\cdot N(\vec{r}_2;\vec{r}_2')\,d\vec{r}_2\end{aligned} \tag{16}$$

and

$$\vec{G}(\vec{r}_1)=-\int d\vec{r}_2\cdot h_{12}\cdot P_{12}^r\cdot\vec{S}(\vec{r}_2;\vec{r}_2'). \tag{17}$$

Here h_1 is the one particle operator, h_{12} the two particle operator and P_{12}^r the permutation operator which interchanges $\vec{r}_1$ and $\vec{r}_2$.

The total energy is:

$$\begin{aligned}E=E_0&+\int h_1N(\vec{r}_1;\vec{r}_1')\,d\vec{r}_1+\frac{1}{2}\int h_{12}N(\vec{r}_1;\vec{r}_1')N(\vec{r}_2;\vec{r}_2')\,d\vec{r}_1\,d\vec{r}_2\\ &-\frac{1}{4}\int h_{12}N(\vec{r}_1;\vec{r}_2')N(\vec{r}_2;\vec{r}_1')\,d\vec{r}_1\,d\vec{r}_2-\int h_{12}\vec{S}(\vec{r}_1;\vec{r}_2')\cdot\vec{S}(\vec{r}_2;\vec{r}_1')\,d\vec{r}_1\,d\vec{r}_2.\end{aligned} \tag{18}$$

Using this general framework we now study the one-dimensional δ-function system for each one of the eight Fukutome classes.

2.1. RHF (TICS) *State*

In this case we have the set (9) of orbitals in the doubly filled scheme:

$$\begin{aligned}&\eta(k_1, z)\alpha(\zeta), \eta(k_2, z)\alpha(\zeta), \ldots, \eta(k_{N/2}, z)\alpha(\zeta)\\&\eta(k_1, z)\beta(\zeta), \eta(k_2, z)\beta(\zeta), \ldots, \eta(k_{N/2}, z)\beta(\zeta)\end{aligned} \tag{19}$$

with

$$-\frac{\pi}{2a} \leq k_i < \frac{\pi}{2a}$$

$$-m \leq \kappa_i \leq m.$$

From Eqs. (10)–(12) we get:

$$N^{(\mathrm{RHF})}(z_2; z_2') = 2\frac{\sin(\pi n/2)(z_2 - z_2')}{\pi(z_2 - z_2')} \tag{20}$$

$$S_x(z_2; z_2') = S_y(z_2; z_2') = S_z(z_2; z_2') = 0. \tag{21}$$

From Eq. (15) and the equation:

$$\mathcal{H}_{\mathrm{eff}}^{(\mathrm{RHF})}(z_1)\eta(k, z_1) = \epsilon_k \eta(k, z_1) \tag{22}$$

replacing h_{12} by our model potential (1) we get for the one electron energy:

$$\epsilon_k = \tfrac{1}{2}k^2 - \tfrac{1}{2}\gamma \cdot n. \tag{23}$$

2.2. CCW-*State*

We introduce a translation q so far undetermined, in momentum space. The CCW pairing [29] is:

$$\begin{cases}\phi(k, z)\alpha = (\eta(k, z) \cdot u_k + \eta(k + q, z) \cdot v_k)\alpha\\ \phi'(k, z)\beta = (\eta(k, z) \cdot u_k + \eta(k + q, z) \cdot v_k)\beta\end{cases} \tag{24}$$

with the convention: if $k < 0$, $q > 0$ and if $k > 0$, $q < 0$. The choice $q = \pi/a$ corresponds to the "vertical pairing", which means that in the reduced zone scheme we mix states with the same k, one of which is occupied and the other unoccupied in RHF.

We keep a general q and study how the choice of q affects the gap and the total energy of the system.

In order to avoid non-orthogonality complications we exclude values of q such that $|q| < \pi/a$.

From Eqs. (10), (11), (12) and (24) we get:

$$N^{(\mathrm{CCW})}(z_1, z_1) = n + \frac{4\cos qz_1}{L} \sum_{\kappa=-m}^{m} u_k v_k \tag{25}$$

$$S_x^{(\mathrm{CCW})}(z_1; z_1') = S_y^{(\mathrm{CCW})}(z_1; z_1') = S_z^{(\mathrm{CCW})}(z_1; z_1') = 0. \tag{26}$$

For the gap equation [30, 31] we need

$$\frac{\lambda_k}{\sqrt{(1-\lambda_k^2)}} \cdot \Delta_k = \tilde{\tilde{\varepsilon}}_k - \tilde{\varepsilon}_k \tag{27}$$

$$\Delta_k^{(\mathrm{CCW})} = -\int \mathscr{H}_{\mathrm{eff}}^{(\mathrm{CCW})}(z_1)[\eta(k, z_1)\eta^*(k+q, z_1') + \eta(k+q, z_1)\eta^*(k, z_1')]\, dz_1 \tag{28}$$

$$\tilde{\varepsilon}_K^{(\mathrm{CCW})} = \int dz_1\, \mathscr{H}_{\mathrm{eff}}^{(\mathrm{CCW})}(z_1)\eta(k, z_1)\eta^*(k, z_1') \tag{29}$$

$$\tilde{\tilde{\varepsilon}}_k^{(\mathrm{CCW})} = \int dz_1\, \mathscr{H}_{\mathrm{eff}}^{(\mathrm{CCW})}(z_1)\eta(k+q, z_1)\eta^*(k+q, z_1). \tag{30}$$

From Eqs. (15), (24), (25) and (28) we get:

$$\Delta = \Delta_k^{(\mathrm{CCW})} = \frac{2\gamma}{L} \sum_{\kappa'=m}^{m} u_{k'} \cdot v_{k'} = \gamma_{\bar{L}} \sum_{\kappa'=-m}^{m} \sqrt{1-\lambda_{\kappa'}} \tag{31}$$

which shows that in this case the gap does not depend on k. We get further from (29) and (30):

$$\tilde{\tilde{\varepsilon}}_k^{(\mathrm{CCW})} - \tilde{\varepsilon}_k^{(\mathrm{CCW})} = \tfrac{1}{2}q(2k+q). \tag{32}$$

Combining Eqs. (31) and (32) with Eq. (27) we get the gap equation

$$\Delta = \gamma L^{-1} \sum_{\kappa=-m}^{m} \sqrt{\frac{\Delta^2}{\Delta^2 + \frac{1}{4}q^2(2k+q)^2}} \tag{33}$$

which has to be solved numerically. The solution of Eq. (33) becomes easier if we use the fact that N is very large and convert the summation to an integration.

For the total energy, from Eq. (18) we get (with $\gamma = 1$)

$$E_{\mathrm{CCW}} - E_{\mathrm{RHF}} = \sum_{\kappa=-m}^{m} \tfrac{1}{2}(2k+q)(1-\lambda_k) - \tfrac{1}{2}L\Delta^2. \tag{34}$$

2.2. ASW *State*

The corresponding pairing is:

$$\begin{cases} \phi(k, z)\alpha = (\eta(k, z) \cdot u_k + \eta(k+q, z) \cdot v_k)\alpha \\ \phi'(k, z)\beta = (\eta(k, z) \cdot u_k - \eta(k+q, z) \cdot v_k)\beta \end{cases} \tag{35}$$

with the same convention for q as in (b), and with the restriction $|q| \geq \pi/a$

From Eqs. (10), (11), (12) and (35) we get:

$$N^{(\mathrm{ASW})}(z_1, z_1) = n \tag{36}$$

and

$$S_x^{(\mathrm{ASW})}(z_1, z_1) = S_y^{(\mathrm{ASW})}(z_1, z_1) = 0 \tag{37}$$

$$S_z^{(\mathrm{ASW})}(z_1, z_1) = \frac{2\cos qz}{L} \sum_{\kappa=-m}^{m} u_k \cdot v_k. \tag{38}$$

The gap splits into two parts:

$$\Delta_k^{\alpha(\mathrm{ASW})} = -\int dz_1\, \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{ASW})}(z_1) \cdot [\eta(k, z_1) \cdot \eta^*(k+q, z_1') + \eta(k+q, z_1)\eta^*(k, z_1')] \tag{39}$$

for the α spin orbitals, and

$$\Delta_k^{\beta(\mathrm{ASW})} = +\int dz_1\, \mathscr{H}_{\mathrm{eff}}^{\beta(\mathrm{ASW})}(z_1)[\eta(k, z_1) \cdot \eta^*(k+q, z_1') + \eta(k+q, z_1)\eta^*(k, z_1')] \tag{40}$$

for the β-spin orbitals and where $\mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{ASW})}$ and $\mathscr{H}_{\mathrm{eff}}^{\beta(\mathrm{ASW})}$ are the α and β components of the effective operator (15), respectively.

We have also:

$$\tilde{\varepsilon}_k^{\alpha(\mathrm{ASW})} = \int \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{ASW})}(z_1) \cdot \eta(k, z_1)\eta^*(k, z_1')\, dz_1 \tag{41}$$

$$\tilde{\tilde{\varepsilon}}_k^{\alpha(\mathrm{ASW})} = \int \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{ASW})}(z_1) \cdot \eta(k+q, z_1)\eta^*(k+q, z_1')\, dz_1 \tag{42}$$

with similar expressions for the β components. From (15), (35), (36), (37), (38), (39), (40) we get:

$$\Delta_k^{\alpha(\mathrm{ASW})} = \Delta_k^{\beta(\mathrm{ASW})} \equiv \Delta^{(\mathrm{ASW})} = \frac{2\gamma}{L} \sum_{\kappa=-m}^{m} u_{k'} v_{k'} \tag{43}$$

which is the same as the $\Delta_k^{(\mathrm{CCW})}$ and indeed independent of k. From Eqs. (27), (41), (42), (43) we get:

$$\Delta^{(\mathrm{ASW})} = \frac{\gamma}{L} \sum_{\kappa=-m}^{m} \sqrt{\frac{(\Delta^{(\mathrm{ASW})})^2}{(\Delta^{(\mathrm{ASW})})^2 + \frac{1}{4}q^2(2k+q)^2}} \tag{44}$$

which is identical with the corresponding expression (33) for the $\Delta^{(\mathrm{CCW})}$. For the total energy we get:

$$E_{\mathrm{ASW}} - E_{\mathrm{RHF}} \equiv E_{\mathrm{CCW}} - E_{\mathrm{RHF}}$$

as given by Eqs. (34).

2.4. TSDW-*State*

The corresponding pairing is:

$$\begin{cases} \phi(k, z\zeta) = u_k \cdot \eta(k, z)\alpha(\zeta) + v_k\, \eta^*(k+q, z)\beta(\zeta) \\ \phi'(k, z\zeta) = v_k \cdot \eta(k+q, z)\alpha(\zeta) + u_k \eta^*(k, z)\beta(\zeta) \end{cases} \tag{45}$$

With the same convention for q as in Section 2.1, and with the restriction $|q| \geq \pi/a$.

From Eqs. (10), (11), (12), and (45) we get:

$$N^{(\mathrm{TSDW})}(z_1, z_1) = n \tag{46}$$

$$S_x^{(\mathrm{TSDW})}(z_1, z_1) = \frac{2}{L} \sum_{\kappa=-m}^{m} u_k v_k \cos\left[(2k+q)z_1\right] \tag{47}$$

$$S_y^{(\mathrm{TSDW})}(z_1, z_1) = -\frac{2}{L} \sum_{\kappa=-m}^{m} u_k \cdot v_k \sin\left[(2k+q)z_1\right] \tag{48}$$

$$S_z^{(\mathrm{TSDW})}(z_1, z_1) = 0. \tag{49}$$

The gap is given by:

$$\begin{aligned}\Delta_k^{\alpha(\mathrm{TSDW})} = -\int dz_1\, \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{TSDW})}(z_1, \varphi_1)[\eta(k, z_1)\eta^*(k+q, z_1')\alpha(\zeta_1)\beta(\zeta_1') \\ + \eta(k+q, z_1)\eta^*(k, z_1')\alpha(\zeta_1)\beta(\zeta_1')].\end{aligned} \tag{50}$$

From Eqs. (15) and (45) we get:

$$\Delta_k^{\alpha(\mathrm{TSDW})} = \frac{4\gamma}{L} u_k v_k \tag{51}$$

which exhibits an explicit k-dependence of the gap $\Delta_k^{(\mathrm{TSDW})}$.

We have also:

$$\tilde{\varepsilon}_k^{\alpha(\mathrm{TSDW})} = \int dz_1\, d\zeta_1 \cdot \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{TSDW})}(z_1, \zeta_1)\eta(k_1 z_1)\eta^*(k+q, z_1')\alpha(\zeta_1)\alpha(\zeta_1') \tag{52}$$

$$\tilde{\tilde{\varepsilon}}_k^{\alpha(\mathrm{TSDW})} = \int dz_1\, d\zeta_1\, \mathscr{H}_{\mathrm{eff}}^{\alpha(\mathrm{TSDW})}(z_1, \zeta_1)\eta^*(k+q, z_1)\eta(k+q, z_1)\beta(\zeta_1)\beta(\zeta_1'). \tag{53}$$

The expressions for β-components are exactly the same. From Eqs. (27), (51), (52), (53)

$$\lambda_k^{(\mathrm{RSDW})} = \frac{L}{2} \cdot \frac{1}{2}(2k+q) \cdot q. \tag{54}$$

For the total energy we get (with $\gamma = 1$):

$$\begin{aligned}E_{\mathrm{TSDW}} - E_{\mathrm{RHF}} = \frac{1}{3}\left(\frac{\pi}{2a}\right)^2 \cdot N + \sum_{\kappa=-m}^{m} \tfrac{1}{2}(1-\lambda_k)q(2k+q) \\ -\frac{4}{L}\left(\sum_{\kappa=-m}^{m} \tfrac{1}{2}\sqrt{1-\lambda_k}\right)^2.\end{aligned} \tag{55}$$

2.5. TSDW$_1$-*State*

By this we mean the state obtained in Overhauser's way [9, 10]:

$$\begin{cases}\phi(k, z\zeta) = u_k \cdot \eta(k, z)\alpha(\zeta) + v_k \cdot \eta(k+q, z)\beta(\zeta) \\ \phi'(k, z\zeta) = u_k \cdot \eta(k, z)\beta(\zeta) - v_k \cdot \eta(k-q, z)\alpha(\zeta)\end{cases} \tag{56}$$

where q is kept positive for all k, and with $|q| \geq \pi/a$.

For the number and spin density matrices we get:

$$N^{(\mathrm{TSDW}_1)}(z_1, z_1) = n \tag{57}$$

$$S_x^{(\mathrm{TSDW}_1)}(z_1, z_1) = \frac{2}{L}(\cos qz_1) - \sum_{\kappa=-m}^{m} u_k v_k \tag{58}$$

$$S_y^{(\mathrm{TSDW}_1)}(z_1, z_1) = \frac{2}{L}(\sin qz_1) \sum_{\kappa=-m}^{m} u_k v_k \tag{59}$$

$$S_z^{(\mathrm{TSDW}_1)}(z_1, z_1) = 0. \tag{60}$$

The gap can be split into two parts: for the "spin-up" part and "spin-down" part in Overhauser's sense, a terminology suggested by the pairing (56), where the α spin plane waves are mixed with states to the right of the chosen k-value and the β-spin plane waves are mixed with states to the left.

Using the same procedure as in the previous cases we get:

"spin up":

$$\begin{aligned}\Delta_k^{\alpha(\mathrm{TSDW}_1)} = &\int dz_1\, dz_2\, \gamma[S_x(z_1, z_1) + iS_y(z_1, z_1)]\eta(k_1, z_1)\eta^*(k+q, z_1) \\ &+ \int dz_1\, dz_2\, \gamma[S_x(z_1, z_1) - iS_y(z_1, z_1)]\eta(k+q, z_1)\eta^*(k, z_1)\end{aligned} \tag{61}$$

"spin down":

$$\begin{aligned}\Delta_k^{\beta(\mathrm{TSDW}_1)} = &\int dz_1\, dz_2\, \gamma[S_x(z_1, z_1) + iS_y(z_1, z_1)]\eta^*(k, z_1)\eta(k-q, z_1) \\ &+ \int dz_1\, dz_2\, \gamma[S_x(z_1, z_1) - iS_y(z_1, z_1)]\eta^*(k-q, z_1)\eta(k, z_1)\end{aligned} \tag{62}$$

both of which lead to the same expression:

$$\delta = \Delta_k^{\alpha(\mathrm{TSDW}_1)} = \Delta_k^{\beta(\mathrm{TSDW}_1)} = \frac{4\gamma}{L} \sum_{\kappa=-m}^{m} u_{k'} \cdot v_{k'}. \tag{63}$$

For the gap equation we get:

$$\delta = \frac{2\gamma}{L} \sum_{\kappa=-m}^{m} \sqrt{\frac{\delta^2}{\delta^2 + \frac{1}{4}q^2(2k+q)^2}}. \tag{64}$$

For the total energy, always with $\gamma = 1$ we get:

$$E_{\mathrm{TSDW}_1} - E_{\mathrm{RHF}} = \frac{1}{2} \sum_{\kappa=-m}^{m} k^2 + q^2 \sum_{\kappa=-m}^{m} \tfrac{1}{2}(1-\lambda_k) - \tfrac{1}{4}\delta^2 \cdot L. \tag{65}$$

3. Numerical Solutions and Discussions

We have solved Eqs. (33) and (64) numerically for the fixed value $\gamma = 1$ for different q and different densities $n = 1/a$. Atomic units are used throughout. In Fig. 1 and Fig. 2 we show the dependence of the gap on q and a. The important result is that broken symmetry states do not exist for all possible values of q. One finds instead only an interval, the length of which is dependent on the electronic density. This feature seems natural because beyond the just mentioned interval the weight of those mixed states which differ too much in their energies becomes dominant.

The gap, for both cases decreases with the increase of q within the relevant interval for any electronic density.

In Sect. 2 we mentioned only CCW, ASW, TSDW and TSDW$_1$ states. But if we let $q = \pi/a$ then the complex conjugation operator becomes a symmetry

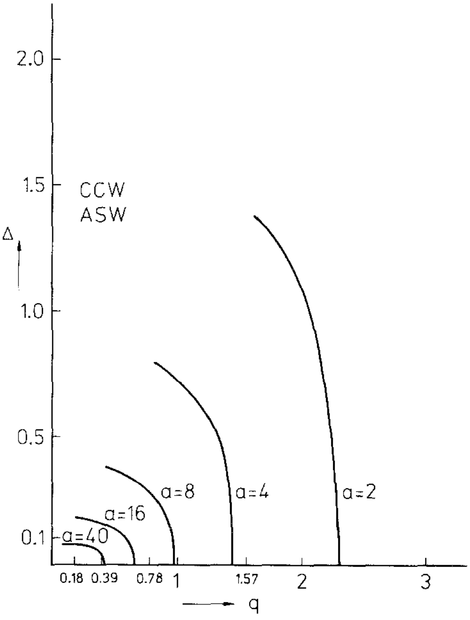


Fig. 1. The gap Δ as a function of q for different densities (Δ, q in atomic units)

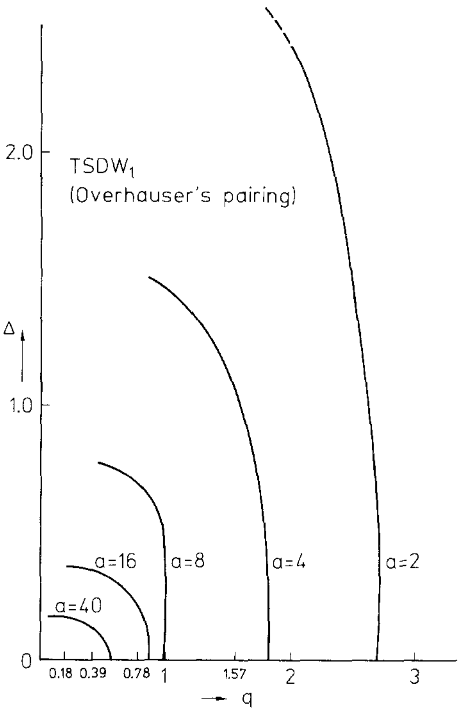
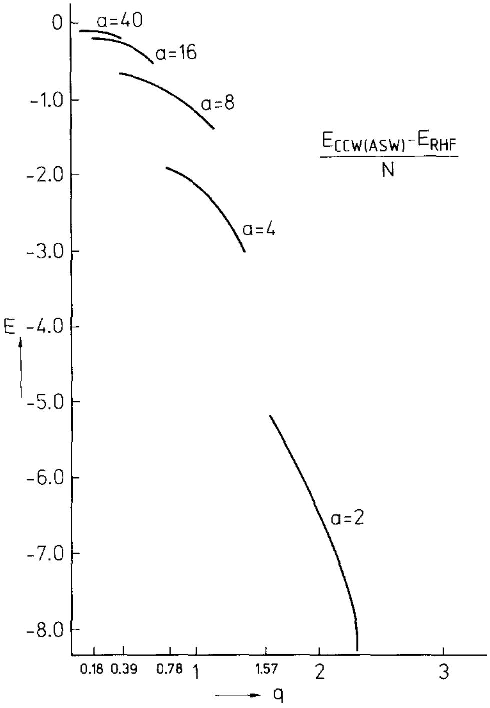


Fig. 2. The gap as a function of q for different densities (Δ, q in atomic units)



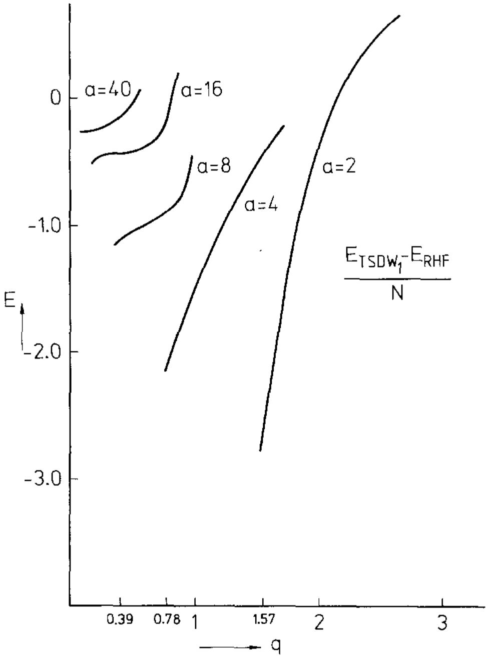


Fig. 3. The difference of energy per particle in the CCW (ASW)-state w.r. to RHF one as a function of q for different densities (E, q in atomic units)

Fig. 4. The difference of energy per particle in the TSDW$_1$-state w.r. to RHF one as a function of q for different densities (E, q in atomic units)

element and CCW becomes a TICS (CDW) state and ASW becomes ASDW or the AMO state.

In Figs. 3 and 4 we show the difference of the energy per electron of the broken symmetry state with the reference, RHF-state, as a function of the mixing parameter q and for different values of the electronic density. Whereas the CCW (CDW) state in the relevant interval is always more stable than RHF for all densities, for TSDW$_1$ this is not the case. For some q, and for small and large densities, TSDW$_1$ exists, but becomes less stable than the RHF-state, in agreement with Overhauser's qualitative comments [10]. It is known that the AMO and SDW states for the electron gas with δ-function interaction exist for all values of γ [9, 11]. In the just mentioned references it is stated also, without actual calculation that $q = \pi/a$, or the "vertical pairing" is the best one. This agrees with our results.

We also notice the different behaviour of the stability of CCW (CDW) state (which has the same energy as ASW (AMO) state which increases with the increase of q, in contradiction of the stability of TSDW-state which decreases when q increases.

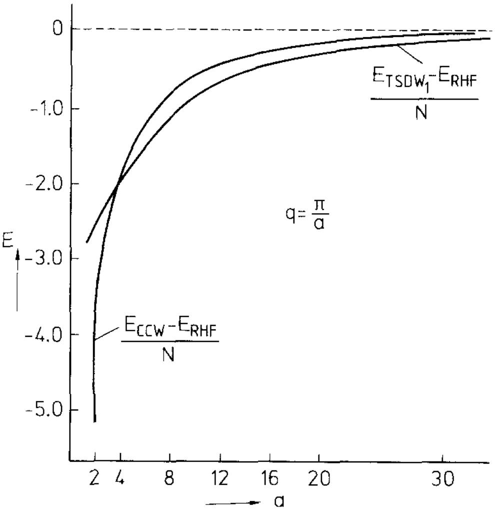


Fig. 5. The differences of total energies w.r. to RHF as functions of a for $q=\pi/q$ (E, a in atomic units)

The interesting thing is that for $q=\pi/a$, the ASDW (AMO) or CDW-state and also the TSDW$_1$-state exist and have lower energy then the reference RHF-state. In Fig. 5 we show the dependence of mentioned energy differences of ASDW and TSDW$_1$ on the electronic density for the value $q=\pi/a$. It is found that for $a \simeq 3.8$ a.u. we have a transition, the TSDW$_1$ state becomes more stable than the AMO state.

We notice also that the degeneracy between the CCW and ASW is due to the particular δ-potential we have chosen and that the assumption of the cancellation of the attraction to the positive background with the background–background interaction becomes more questionable in the CCW (CDW)-state.

Finally, the state TSDW, shows up only for $q=0$, as it is seen from Eq. (54), because for all other q we get λ_k outside the interval $(-1, 1)$. But, as is clear from Eq. (55) the reference RHF-state is more stable than TSDW-state.

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