Symmetry breaking in the self-consistent Kohn-Sham equations

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Abstract

The Kohn-Sham (KS) equations determine, in a self-consistent way, the particle density of an interacting fermion system at thermal equilibrium. We consider a situation when the KS equations are known to have a unique solution at high temperatures and this solution is a uniform particle density. We show that, at zero temperature, there are stable solutions that are not uniform. We provide the general principles behind this phenomenon, namely the conditions when it can be observed and how to construct these non-uniform solutions. Two concrete examples are provided, including fermions on the sphere which are shown to crystallize in a structure that resembles the C_{60} molecule.

1 Introduction

We consider a system of N interacting fermions in a finite volume. Since we want to avoid the surface effects, we actually consider the fermions moving on toruses and spheres, or, more generally, on a closed Riemann manifold $\mathcal{M}$ of finite volume Ω. According to the Kohn-Sham theory [1] (and later extensions), the particle density at thermal equilibrium at a temperature T ($\beta = 1/kT$) is a solution of the following set of equations:

$$(H_0 + V_n)\phi_i = \epsilon_i \phi_i$$

$$n(x) = \sum_i \left(1 + e^{\beta(\epsilon_i - \mu)}\right)^{-1} |\phi_i(x)|^2, \tag{1}$$

with V_n an effective potential depending entirely on the particle density n and μ determined from $\int n(x)dx = N$. H_0 is the single particle, non-interacting Hamiltonian. We refer to $H_n \equiv H_0 + \lambda V_n$ as the Kohn-Sham Hamiltonian, where we introduced the coupling constant λ for convenience. We will neglect the spin degree of freedom.

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The effective potential is not known, more precisely, there is no direct and constructive algorithm or prescription which could, at least in principle, lead to the exact V_n. However, for the electron gas at least, there is a set of very successful approximations of V_n, which already provide numerical results that are within the so called "chemical precision" [2]. Although in this paper we do not use a specific approximation, we will often make reference to two approximations in order to check our assumptions. These approximations are the Local Density Approximation (LDA): $V_n = v*n+v_{xc}(n)$ (v the two body interaction), i.e. V_n is the sum between the Hartree potential and a *function* of density, and the quadratic approximation (QA): $V_n = K*n$, i.e. V_n is the convolution of the density with a certain kernel. The mathematical structure of QA is the same as that of the Hartree approximation.

In this paper, we are not concerned with the physical and mathematical principles leading to the KS equations, but rather with the mathematical structure of these equations, in particular with the question of uniqueness at zero temperature.

Let us discuss first what it is known at finite temperature. Assume the following:

A1) H_0 is self adjoint, bounded from below; the kernel $(H_0+a)^{-2}(x,x')$ is continuous and
$$k_a = \sup_{x\in\mathcal{M}} (H_0+a)^{-2}(x,x) < \infty.$$

A2) $V_n \in L^2(\mathcal{M})$ and $w \equiv \sup \|V_n\|_{L^2} < \infty$, where the supremum is taken over all n in
$$S^N \equiv \{n \in L^1(\mathcal{M}),\ \|n\|_{L^1} = N\}.$$

As H_0 is in general equal to minus the Laplace operator, A1 is easy to check for 1, 2 and 3 dimensional toruses or spheres. It fails in 4 and higher dimensions. Since $\mathcal{M}$ is of finite volume, A1 automatically implies that $\exp(-\beta H_0)$ is trace class. A1 also implies that $\|f\|_{L^\infty} \leq \sqrt{k_a}\|(H_0+a)f\|_{L^2}$ (with equality when $f(x) = (H_0+a)^{-2}(x,x_0)$!). Together with A2 (easy to verify for LDA and QA , see Refs. [3, 4]), this leads to

$$\|V_n(H_0+a)^{-1}\| \leq w\sqrt{k_a} \equiv \gamma_a. \tag{2}$$

Then, H_n is self-adjoint for all $n \in S^N$ and, as it follows from Ref. [3], the Kohn-Sham equations can be formulated as a fixed point problem:

Theorem 1 For $T > 0$, the following map is well defined:

$$T : S^N \to S^N$$
$$S^N \ni n \to T[n](x) = \left(1 + e^{\beta(H_n-\mu)}\right)^{-1}(x,x), \tag{3}$$

where μ is the unique solution of $N = Tr\left(1+e^{\beta(H_n-\mu)}\right)^{-1}$. The fixed points of T generate all possible solutions of the KS equations.

Many will recognize in Eq. (3) the usual formulation of the KS problem in terms of the density matrix. When appealing to the fixed point theorem, the functional form of the map T and its domain of definition are *equally* important. What is new in the above result is that the density matrix is well defined for all densities which integrate to N.

Apart from complications that can occur at low particle densities and which will not be addressed here, the following assumption can be easily verified for LDA and QA (see Ref. [3, 4]):

A3) There exists $\chi < \infty$ such that

$$\|V_n - V_{n'}\|_{L^1} \leq \chi \|n - n'\|_{L^1},$$

for any n, $n' \in S^N$.

A3 assures the existence of one and only one fixed point of T for λ smaller than a critical value λ_c. Supposing that A1-A3 holds uniformly at any temperature, it is not hard to show that λ_c increases with temperature. In other words, if λ is kept fixed, A1-A3 guaranties the existence of a unique fixed point of T at high temperatures.

The situation at zero temperature is more delicate. The density now becomes $n(x) = \sum |\phi_i(x)|^2$ where the sum goes over the lowest N energy states of H_n. If the last occupied energy level is degenerate and only partially occupied, there is an ambiguity in defining $n(x)$. We deal exactly with this situation.

Let us assume that that there is a continuous group G_c acting ergodically on $\mathcal{M}$ and preserving the Riemann structure. On torus or sphere, this group will be simply the translations or rotations. Let us consider the natural unitary representation of G_c in $L^2(\mathcal{M})$:

$$G_c \ni g \to \hat{g},\ (\hat{g}f)(x) = f(gx).$$

We assume that H_0 commutes with all $\hat{g}$ and that every symmetry of the particle density is automatically a symmetry of the effective potential:

A4) If $n(gx) = n(x)$, then $V_n(gx) = V_n(x)$ $(\hat{g}V_n\hat{g}^{-1} = V_n)$.

This assumption can be easily verified for LDA and QA. Besides other things, A4 implies that V_n is a constant if $n(x)$ is uniform, and we can fix this constant to zero. In other words, the Kohn-Sham Hamiltonian reduces to H_0 if $n(x) = \bar{n}$ $(\bar{n} = N/\Omega)$. Then, it is trivial to show that, at any finite temperature, $\bar{n}$ is a solution of the KS equations. With our assumptions, we also know that this is the only solution at high temperatures. At zero temperature, assume that, if we populate with N particles the energy levels of H_0, from smaller to higher energies, we end up with N_0 particles on the last occupied energy level, assumed d-fold degenerate with $d > N_0$. We refer to this level and its energy as the Fermi level and Fermi energy ϵ_F. If we can find N_0 states at the Fermi level so as to generate a uniform particle density, then $\bar{n}$ is a solution of the KS equations. If there is no such combination of states, than either there is no solution or the solution is not uniform.

We now show when and how these non-uniform solution can be found. We look for a finite subgroup G of G_c, which has to satisfy two simple conditions. We index its irreducible representations by Γ and use the symbol $|\Gamma|$ to specify their dimension. Let P_Γ denote the projectors

$$P_\Gamma = \frac{|\Gamma|}{|G|} \sum_{g \in G} \chi_\Gamma(g) \hat{g},$$

with the following properties

$$P_\Gamma P_{\Gamma\prime} = \delta_{\Gamma\Gamma\prime}, \quad \sum_\Gamma P_\Gamma = I.$$

Above, $|G|$ denotes the cardinal of G and $\chi_\Gamma(g)$ the character of g in the representation Γ. The group G must satisfy the following:

A5) If $\mathcal{H}_F$ denotes the eigenspace of H_0 corresponding to ϵ_F, then $\mathcal{H}_F = \oplus_i P_{\Gamma_i}\mathcal{H}_F$ with $\dim P_{\Gamma_i}\mathcal{H}_F = |\Gamma_i|$, i.e. we have irreducible representations of G in each $P_{\Gamma_i}\mathcal{H}_F$.

A6) $|\Gamma_i| = N_0$ for some i (we rearrange so that $i = 0$).

Let now $n_0(x)$ be the particle density when we populate all the states of H_0 below ϵ_F plus the N_0 states in $P_{\Gamma_0}\mathcal{H}_F$. The last condition is on the effective potential:

A7) If $V_{\Gamma_i} \equiv \langle \phi^0_{\Gamma_i}, V_{n_0}\phi^0_{\Gamma_i}\rangle$ with $\phi^0_{\Gamma_i}$ any norm one vector from $P_{\Gamma_i}\mathcal{H}_F$, then $V_{\Gamma_i} - V_{\Gamma_0} > 0$ for all $i > 0$.

If the subgroup G satisfying A5-A6 exists and the effective potential satisfies A7, then, at least for small coupling constants, the zero temperature KS equations have a non-uniform solution $n(x) = n_0(x) + o(\lambda)$. This is our main result.

2 The Proof

We restrict the search for $n(x)$ to the densities that are symmetric relative to G. To define this space precisely, we consider the isometries

$$T_g : L^1(\mathcal{M}) \to L^1(\mathcal{M}), \quad (T_g n)(x) = n(gx),$$

and define

$$L^1_{sym} \equiv \bigcap_{g \in G} Ker(T_g - I).$$

It is important to notice that L^1_{sym} is a closed subspace of $L^1(\mathcal{M})$. Since the solutions of the KS equations are not effected if we add a constant to V_n, we can assume without loosing generality that $V_{\Gamma_0} < 0$, $V_{\Gamma_i} > 0$ for $i > 0$ and $\min_{i>0} V_{\Gamma_i} = |V_{\Gamma_0}|$.

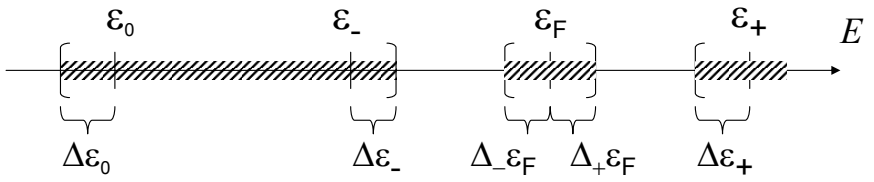

Figure 1: If ϵ_0 and $\epsilon_{\mp}$ denote the ground state and energy levels below/above ϵ_F of H_0, then, at small λ, the spectrum of H_n ($n \in S^N$) is contained in $\mathcal{I}$ (the hachured region of the real axis), where: $\Delta\epsilon_0 = \lambda\gamma_a(\epsilon_0 + a)$, $\Delta\epsilon_- = \frac{\lambda\gamma_a}{1-2\lambda\gamma_a}(\epsilon_- + a)$, $\Delta_-\epsilon_F = \lambda\gamma_a(\epsilon_F + a)$, $\Delta_+\epsilon_F = \frac{\lambda\gamma_a}{1-2\lambda\gamma_a}(\epsilon_F + a)$ and $\Delta\epsilon_+ = \lambda\gamma_a(\epsilon_+ + a)$

Theorem 2 Let us consider the closed subset of $L^1(\mathcal{M})$,

$$S^{N,\epsilon}_{sym} \equiv \{n \in L^1_{sym},\ \|n\|_{L^1} = N,\ \|n - n_0\|_{L^1} \leq \epsilon\}.$$

Then, for ϵ and λ small enough:

i) The following map is well defined

$$T_\epsilon : S^{N,\epsilon}_{sym} \to S^{N,\epsilon}_{sym},\ T_\epsilon[n](x) = P^<_n(x,x),$$

where $P^<_n$ denotes the spectral projector of H_n onto the spectrum below ϵ_F (without including ϵ_F).

ii) The fixed points of T_ϵ are solutions of the KS equations.

iii) T_ϵ has one and only one fixed point.

Proof i) Let us show first that T_ϵ takes $S^{N,\epsilon}_{sym}$ into L^1_{sym}. We notice that $P^<_n$ is well defined for all $n \in S^{N,\epsilon}_{sym}$ and can be determined from the resolvent of H_n. Also, A1-A2 guaranties that the kernel of $P^<_n$ is continuous, thus its diagonal is well defined. From A4, H_n and consequently $P^<_n$ commutes with all $\hat{g}$, $g \in G$, for all $n \in S^{N,\epsilon}_{sym}$. Then

$$T_\epsilon[n](gx) = P^<_n(gx, gx) = (\hat{g}P^<_n\hat{g}^{-1})(x,x) = T_\epsilon[n](x).$$

Next, we show that T_ϵ takes $S^{N,\epsilon}_{sym}$ into S^N. For this, we need to show that H_n has exactly N states below ϵ_F, for all $n \in S^{N,\epsilon}_{sym}$. For λ small, a first, rough location of the spectrum can be obtained from Eq. (2). An elementary argument will show that the spectrum of H_n is always located inside the set $\mathcal{I}$ defined and shown in Fig. 1. We now investigate the splitting of the Fermi level. For any $n \in S^{N,\epsilon}_{sym}$, the Fermi level will split in sub-levels, each corresponding to the

different irreducible representations Γ_i (see A5). The energy of any such level can be computed as

$$E_\Gamma(n) = \frac{1}{|\Gamma|} Tr P_\Gamma \int_{\gamma'} z(z - H_n)^{-1} \frac{dz}{2\pi i},$$

with γ' the contour described in Fig. 2. Simple manipulations leads to:

$$E_\Gamma(n) = \epsilon_F + \lambda \langle \phi^0_\Gamma, V_n \phi^0_\Gamma \rangle + \lambda^2 \beta_{\Gamma,\lambda}(n), \tag{4}$$

with ϕ^0_Γ any norm one vector from $P_\Gamma \mathcal{H}_F$ and

$$\beta_{\Gamma,\lambda}(n) = \frac{1}{|\Gamma|} Tr P_\Gamma \int_{\gamma'} z(z - H_0)^{-1} V_n (z - H_n)^{-1} V_n (z - H_0)^{-1} \frac{dz}{2\pi i}.$$

We have an upper bound, $\beta_{\Gamma,\lambda}(n) \leq \bar{\beta}$, with $\bar{\beta}$ independent of Γ, λ or n:

$$\begin{aligned} \beta_{\Gamma,\lambda}(n) &\leq 2 \int_{\gamma'} |z| \| (z - H_0)^{-1} V_n (z - H_n)^{-1} V_n (z - H_0)^{-1} \| \frac{|dz|}{2\pi} \\ &\leq \frac{2\gamma_a^2}{\Delta} \int_{\gamma'} |z| \left(1 + \frac{|z + a|}{\Delta} \right)^2 \frac{|dz|}{2\pi}. \end{aligned} \tag{5}$$

Notice also that

$$\langle \phi^0_\Gamma, V_n \phi^0_\Gamma \rangle = V_\Gamma + \int [V_n(x) - V_{n_0}(x)] |\phi^0_\Gamma(x)|^2 dx.$$

Using the eigenvectors expansion of $(H_0 + a)^{-2}$, one can derive

$$|\phi^0_\Gamma(x)|^2 \leq (\epsilon_F + a)^2 k_a,$$

leading to

$$|\langle \phi^0_\Gamma, V_n \phi^0_\Gamma \rangle - V_\Gamma| \leq (\epsilon_F + a)^2 k_a \chi \epsilon. \tag{6}$$

Returning to Eq. (4), it follows from Eqs. (5) and (6) that $E_{\Gamma_0} < \epsilon_F$ and $E_\Gamma > \epsilon_F$ for $\Gamma \neq \Gamma_0$, as long as

$$\epsilon < \frac{|V_{\Gamma_0}| - \lambda \bar{\beta}}{(\epsilon_F + a)^2 k_a \chi}. \tag{7}$$

The last thing we need to show is that

$$\| T_\epsilon[n] - n_0 \|_{L^1} \leq \epsilon. \tag{8}$$

Let us consider

$$\hat{Z}[n] = \int_\gamma (z - H_n)^{-1} \frac{dz}{2\pi i} + P_{\Gamma_0} \int_{\gamma'} (z - H_n)^{-1} \frac{dz}{2\pi i}, \tag{9}$$

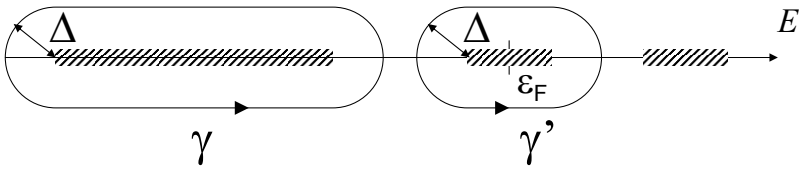

Figure 2: The two contours of integration, γ and γ', surround the states below ϵ_F, respectively the states which have split from the Fermi level such that the distance from any point on the contours to $\mathcal{I}$ is equal to some Δ.

defined on the entire S^N. Based on the previous results, we observe that $P_n^< = \hat{Z}[n]$ for $n \in S^{N,\epsilon}_{sym}$ and ϵ satisfying Eq. (7). Also, notice that $n_0(x) = \hat{Z}[\bar{n}](x,x)$. Moreover, if $\| \ \|_1$ denotes the trace norm,

$$\|\hat{Z}[n] - \hat{Z}[n']\|_1 \leq \frac{\lambda\alpha\chi k_a}{(1-\lambda\gamma_a)^2}\|n - n'\|_{L^1} \tag{10}$$

with

$$\alpha = \left(\int_\gamma + \int_{\gamma'}\right)\left(1 + \frac{|z+a|}{\Delta}\right)^2 \frac{|dz|}{2\pi}.$$

Indeed, let

$$B \equiv (H_0 + a)^{-1}(V_n - V_{n'})(H_0 + a)^{-1}, \tag{11}$$

and $g_{a,z}(t) \equiv (t+a)/(z-t)$. After simple manipulations,

$$\hat{Z}[n] - \hat{Z}[n'] = \lambda\left(\int_\gamma \frac{dz}{2\pi i} + P_{\Gamma_0}\int_{\gamma'}\frac{dz}{2\pi i}\right) g_{a,z}(H_n) \times$$
$$(1 + \lambda(H_0 + a)^{-1}V_n)^{-1} B (1 + \lambda V_{n'}(H_0 + a)^{-1})^{-1} g_{a,z}(H_{n'})$$

and notice that

$$\|g_{a,z}(H_n)\| \leq 1 + \frac{|z+a|}{\Delta}$$

for all $n \in S^N$ and $z \in \gamma$ or γ'. We can conclude at this step that

$$\|\hat{Z}[n] - \hat{Z}[n']\|_1 \leq \frac{\lambda\alpha}{(1-\lambda\gamma_a)^2}\|B\|_1.$$

If we use the polar decomposition $\Delta V = S|\Delta V|$ of $\Delta V \equiv V_n - V_{n'}$, and define $A \equiv |\Delta V|(H_0 + a)^{-1}$, then from Eq. (11)

$$\|B\|_1 = \|A^* S A\| \leq \|A^*\|_{HS}\|SA\|_{HS} \leq \|A\|^2_{HS},$$

and

$$\|A\|_{HS}^2 = \int |\Delta V(x)|(H_0 + a)^{-2}(x,x)dx \leq k_a \chi \|n - n'\|_{L^1}.$$

With Eq. (10) proven, we can easily end the proof of *i)*. Indeed, for all $n \in S_{sym}^{N,\epsilon}$,

$$\begin{aligned} \|T_\epsilon[n] - n_0\|_{L^1} &= \|\hat{Z}[n](x,x) - \hat{Z}[\bar{n}](x,x)\|_{L^1} \\ &\leq \|\hat{Z}[n] - \hat{Z}[\bar{n}]\|_1 \leq \frac{\lambda\alpha\chi k_a}{(1-\lambda\gamma_a)^2}\|n - \bar{n}\|_{L^1} \end{aligned}$$

and

$$\|n - \bar{n}\| \leq \|n - n_0\| + \|n_0 - \bar{n}\| \leq \epsilon + 2N_0.$$

Thus, Eq. (8) is true if

$$\frac{\lambda\alpha\chi k_a(2N_0 + \epsilon)}{(1-\lambda\gamma_a)^2} \leq \epsilon \tag{12}$$

and we remark that Eqs. (7) and (12) can be simultaneously satisfied if λ is small enough.

ii) It follows immediately if we express $P_n^<$ in terms of the eigenvectors and notice that at a fixed point, $n(x) = P_n^<(x,x)$:

$$H_n\phi_i = \epsilon_i\phi_i, \quad n(x) = \sum_{\epsilon_i < \epsilon_F} |\phi_i(x)|^2.$$

Together with $\int n(x)dx = N$, the above equations are exactly the KS equations at zero temperature.

iii) Observe that if we take λ small so the Eq. (12) is satisfied, then

$$\frac{\lambda\alpha\chi k_a}{(1-\lambda\gamma_a)^2} < 1,$$

i.e. $\hat{Z}$ is a contraction. The affirmation follows from the fact that $P_n^<$ and $\hat{Z}[n]$ coincide on $S_{sym}^{N,\epsilon}$ and $S_{sym}^{N,\epsilon}$ is a closed set.

3 Examples

We consider first one of the simplest examples possible: $2N$ particles on a circle of length a. The Kohn-Sham Hamiltonian is $H_n = -\partial_x^2 + V_n$, where x is the coordinate along the circle. The ground state of $H_0 \equiv -\partial_x^2$ is non-degenerate, while all the excited states are doubly degenerate. Thus, if we populate the states of H_0 with $2N$ particles, we end up with one particle occupying a double degenerate energy level, containing the states $a^{-1/2}e^{ik_F x}$ and $a^{-1/2}e^{-ik_F x}$ ($\epsilon_F = k_F^2$).

We now go over the constructions considered in the previous section. The continuous group G_c are the rotations of the circle and the subgroup G can be taken as the identity plus the reflection $r: \ x \to -x$. There are two, one

dimensional irreducible representations of G, $\chi_\pm(r)t = \pm t$. The projectors P_Γ ($\Gamma \to \pm$) are simply given by

$$(P_\pm f)(x) = \frac{1}{\sqrt{2}}[f(x) \pm f(-x)].$$

They decompose $\mathcal{H}_F$ in the invariant spaces

$$P_+\mathcal{H}_F = \{\sqrt{\frac{2}{a}}\cos k_F x\}$$
$$P_-\mathcal{H}_F = \{\sqrt{\frac{2}{a}}\sin k_F x\},$$

each of them providing an irreducible representation for G. Suppose that Γ_0 in A6 is the symmetric (+) representation. In this case, $n_0(x) = \bar{n} + a^{-1}\cos(2k_F x)$ and the non-uniform solution exists if

$$\int V_{n_0}(x)\cos(2k_F x)dx < 0. \tag{13}$$

In LDA, if we approximate $v_{xc}(n_0) \simeq v_{xc}(\bar{n}) + v'_{xc}(\bar{n})(n_0 - \bar{n})$, Eq. (13) reduces to

$$\hat{v}(2k_F) + v'_{xc}(\bar{n}) < 0,$$

where $\hat{v}$ is the Fourier transform of the two-body interaction. For QA, Eq. (13) simply means $\hat{K}(2k_F) < 0$. We will be lead to the same conditions if we choose Γ_0 to be the anti-symmetric (-) representation.

Similar examples can be given for toruses in higher dimensions. We, however, consider the case of fermions on the 2D sphere and show that we can obtain the molecular structure of the C_{60} molecule. In the C_{60} molecule, the carbon atoms seat at the points of intersection between an icosahedron and dodecahedron as shown in Fig. 3a. There are single and double bonds between the carbon atoms. Since the double bond is much stronger than the single bond, we consider C=C as being the building blocks of the C_{60} molecule. In total, there are 30 double bonds and some of them are shown in Fig. 3a. We consider then 30 point particles (of course we have tried 60 particles with no success) on a sphere of radius R, described by $H_n = -R^{-2}\vec{L}^2 + V_n$, where $H_0 = -R^{-2}\vec{L}^2$ is the kinetic energy of a particle on the sphere. The energy levels of H_0 are simply $R^{-2}l(l+1)$, $l = 0,\ 1, \ldots$, and if we populate them in order, we end up with 5 particles on the $l = 5$ level. The continuous group is $O(3)$ and we found that, under the action of the proper icosahedral group, the Fermi level decomposes as

$$\mathcal{H}_F = H_u \oplus T_{1u} \oplus T_{2u},$$

i.e. in a 5 dimensional space plus two 3 dimensional spaces. Thus, the proper icosahedral group satisfies A5-A6 with $\Gamma_0 = H_u$. Then, if the effective potential satisfies A7, the Kohn-Sham equations for the 30 particles on the sphere have a stable solution $n(x) = n_0(x) + o(\lambda)$, where $n_0(x)$ is obtained by populating all $l < 5$ levels plus the 5 states with $l = 5$ and H_u symmetry. This density is shown in Fig. 3b and the resemblance with the C_{60} molecule is evident.

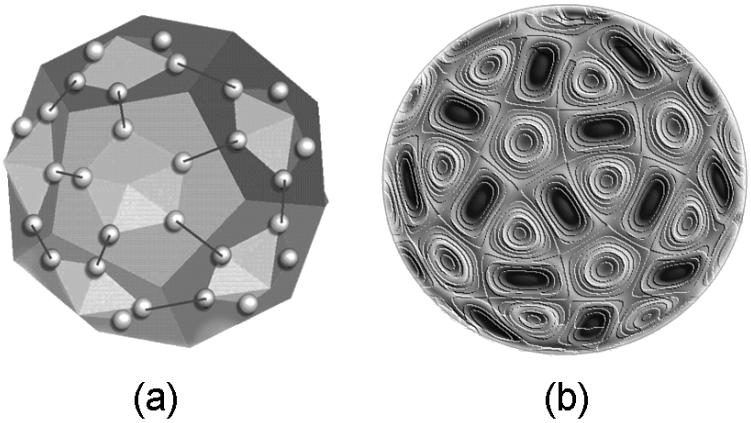

Figure 3: a) The structure of the C_{60} molecule. The small spheres represent the carbon atoms. The double bonds are indicated by segments joining two atoms. b) A contour plot of the density $n_0(x)$ defined in the text. The dark/lighter regions corresponds to high/low densities.

4 Discussion

As opposed to the Jahn-Teller effect [5] or Pierls instability [6], which involves discrete symmetries and the electronic degeneracies are lifted by a displacement of the atoms, the symmetry breaking discussed here involves a continuous group and is due solely to the electron-electron interaction which lifts the electronic degeneracies without any change in the external potential.

There are many numerical studies on this subject. In fact, the modern theory of freezing [7], which can be traced back to the pioneering work of Ramakrishnan and Yussouff [8], is based on the assumption that the liquid-solid transitions occurs because of a bifurcation of the same type as we discussed here. More exactly, the the density of the solid n_s is computed self-consistently as the linear response of the uniform liquid density n_l to the introduction of a density change $\Delta n = n_s - n_l$. In the current state, the procedure cannot predict the lattice symmetry, but rather assumes that the linear response equation has a non-uniform solution, with a prescribed crystalline symmetry (usually known from experiment). Applied to quantum liquids, this procedure is equivalent to solving the Kohn-Sham equations in the quadratic approximation. One can find in Ref. [9] an impressive numerical demonstration of the Wigner crystallization of the electron liquid. For finite systems, we mention Refs. [10] and [11].

We also want to mention that Lieb et al [12] have shown that, for repulsive interactions, the energy levels are always fully occupied in the unrestricted Hartree-Fock approximation, . This result automatically implies that there must

be a symmetry breaking whenever the last occupied level of H_0 is only partially populated. In contradistinction, Ref. [13] showed that, within the Hartree approximation, there is a symmetry breaking for short, attractive interactions. This definitely shows that we have to go beyond the two approximations.

At the end, we want to mention that we have partial but interesting results in the thermodynamic limit and we are currently considering the finite temperature regime.

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