Upper bounds of spin-density wave energies in the homogeneous electron gas

F. Delyon,1,2 B. Bernu,2 L. Baguet,2 and M. Holzmann2,3

1CPHT, UMR 7644 of CNRS, École Polytechnique, F-91128 Palaiseau Cedex, France
2LPTMC, UMR 7600 of CNRS, UPMC, Paris-Sorbonne, F-75252 Paris Cedex 05, France
3LPMMC, UMR 5493 of CNRS, Université J. Fourier, BP 166, F-38042 Grenoble Cedex, France

PACS numbers: 71.10.-w, 71.10.Ca, 71.10.Hf, 71.30.+h, 03.67.Ac

The simplest model of electronic structure is jellium – electrons embedded in a homogeneous background of opposite charge such that the system is neutral. This model is a good starting point to describe properties of simple metals such as sodium[1]. At zero temperature, the only parameter of this model is the density \( n \), or the dimensionless parameter \( r_s = \frac{3}{4\pi n a_B^3} \), where \( a_B = h^2/(m e^2) \) is the Bohr radius. Within the Hartree-Fock approximation (HF), Overhauser has shown that the Fermi gas is unstable under a spin density wave (SDW)[2, 3]. Only recently, almost 50 years after Overhauser’s prediction, explicit numerical estimates of the HF ground state have shown SDW evidences of the electron gas in three[4,7] and two dimensions[7, 8]. Still, a quantitative estimate of the variation of the SDW amplitude and energy in the high density region \( r_s \lesssim 1 \) is missing[9]. In this letter, we generalize Overhauser’s ansatz and provide a quantitative solution of this longstanding problem.

The key point is to search for a solution in a non-perturbative way. Indeed, small domains exist around the Fermi surface where the one-body states differ radically from a single plane wave. These states of wave vector \( \mathbf{k} \) are coupled with the wave vector \( \mathbf{k} + \mathbf{Q}_k \) where \( \mathbf{Q}_k \) is constant over each domain. The larger is this domain, the larger will be the energy gain of the SDWs. One way to enlarge this domain is to cut the top of sphere as explained by Overhauser[2]. In the following we show that adding a small cylinder on the top of the truncated sphere as shown in Fig.1 can increase the energy gain of the SDW by orders of magnitude compared to Overhauser’s ansatz. Furthermore, we provide an explicit estimate of the energy gain of the SDW state. As we will see, the optimal size of these domains dramatically shrinks with increasing density, resulting in an extremely rapid decrease of the tiny SDW energy gain and explaining the difficulties of observing SDW in the high density region.

Our semi-analytical results presented here are compared to recent HF results[6] obtained with periodic models. Indeed, the Overhauser’s ansatz is in fact a periodic model (a crystal where the one-body states are limited to the first mode) as soon as the set vectors \( \mathbf{Q}_k \) belong to a discrete lattice. As the density increases the number of vectors \( \mathbf{Q}_k \) (and of domains around the Fermi sphere) may also increases[2] leading to a quasi-crystal which cannot be describe by a periodic model.

Let us mention that in this paper we focus on the SDW states. These states are easier to compute leading to simpler formulas since the density of charge is constant. Equivalent results may be obtained[2, 3] for the charge density waves (CDW).

In the following, we outline the main steps in the calculation of the SDW energies. First we introduce the deformation of the Fermi surface generalizing Overhauser’s model and describe the SDW ansatz for the single particle states. We then show how the optimal solution can be found by calculating the fixed point solution of a non-linear functional equation. The explicit results are then obtained by restricting to a one dimensional function and compared to the outcome of previous numerical simulations.

Fermi gas energy of the truncated sphere. Let us call \( E_{\text{FG}} \) the HF-energy of the Fermi gas where only plane wave states of wave vectors \( \mathbf{k} \) inside the Fermi sphere of radius \( k_F \) are occupied. Following Overhauser, in a first step the Fermi sphere is deformed into a volume \( \mathcal{F} \) as shown in Fig.1, and its energy increase is denoted \( \Delta E_{\text{FG}} = E_{\text{FG}}^\mathcal{F} - E_{\text{FG}} \). Here, the subscript \( \mathcal{F} \) is used to point out that the many-body state is a Slater determinant of plane wave states inside the corresponding Fermi surface. Using \( k_F \) as unit of wave vectors, the sphere in Fig.1 has unit radius, and the deformation is characterised by a small parameter \( \epsilon \) approaching zero as \( r_s \) decreases. In order to keep the electron density constant, the deformed surface in the figure must be scaled by \( R \) such that \( R^3 \int_{\mathcal{F}} d\mathbf{k} = R^3 \int_{\mathcal{F}} d\mathbf{k} = 4\pi/3 \). The Fermi gas energy per particle in Hartree units \( (\hbar a = \)
The spin density waves. In a second step, the SDW are obtained by replacing a plane wave $|k, \uparrow\rangle$ by $a_k |k, \uparrow\rangle + b_k |k + Q, \downarrow\rangle \langle |ak|^2 + |bk|^2 = 1\rangle$, for $k$ in $F_\gamma$. Symmetrically, for $k$ in $F_\delta$, a plane wave $|k, \downarrow\rangle$ is replaced by the combination $a'_k |k, \downarrow\rangle + b'_k |k + Q, \uparrow\rangle$ with $a'_k = a_{-k}$ and $b'_k = b_{-k}$. We choose $a_k$ real and positive and in the following we assume that $b_k$’s are also positive and that $b_k < a_k^{[12]}$.

As in Fig. 1, $Q_k$ is such that for $k$ in $F_\gamma$, $k + Q$ does not belong to $F_\gamma$, and for $k$ in $F_\delta$, $k + Q$ does not belong to $F_\gamma$. The energy change is given by:

$$\Delta E_{\text{SDW}}^F = \frac{2a_k R^5}{r_s^2} K_{\text{SDW}} - \frac{2a_V R^4}{r_s} V_{\text{SDW}}$$

(5)

$$K_{\text{SDW}} = \int_{F_\gamma} dk \left( ||k + Q||^2 - k^2 \right) b_k^2$$

(6)

$$V_{\text{SDW}} = -\int_{F_\gamma \times F_\gamma} dk dk' \left( \frac{(a_k b_{k'} - b_k a_{k'})^2}{||k - k'||^2} + \frac{(a_k b_{k'} + b_k a_{k'})^2}{||k - k'||^2} \right)$$

(7)

with $k_z = Q - k_z$ (see Fig. 1). Using the linear symmetric operators $T^{\pm}$:

$$(T^\pm f)(k) = \int_{F_\gamma} dk' \left( \frac{1}{||k - k'||^2} \pm \frac{1}{||k - k'||^2} \right) f(k')$$

(8)

Eq. 9 rewrites:

$$\Delta E_{\text{SDW}}^F = \frac{4a_V R^4}{r_s} (2(\kappa, b^2) - (T^- a^2, b^2) - (T^+ ab, ab))$$

(9)

where $(f, g)$ is the scalar product $\int_{F_\gamma} f g$, and $2\kappa(k) = \frac{a_k R}{2a_V r_s} Q(Q - 2k_z) \geq 0$. In Eq. 9, the difference between 1 and $R$ is negligible and in the following we set $R = 1$.

Optimal solution. From the variations of Eq. 9 with respect to $b_k$, the optimal function $b$ satisfies:

$$2b\kappa + b T^-(a^2 - b^2) = \frac{a^2 - b^2}{a} T^+ ab$$

(10)

Setting $\xi = ab$ and using $b^2 \leq \frac{1}{4}$, $a^2 - b^2 = \sqrt{1 - 4\xi^2}$, Eq. 10 rewrites $\xi = J(\xi)$ where:

$$J(\xi) = \frac{1}{2} \frac{T^+ \xi}{\sqrt{(\kappa + T^- \sqrt{1/4 - \xi^2})^2 + (T^+ \xi)^2}}$$

(11)

Thus the point is now to find the fixed points of the operator $J$. The Fermi gas ($\xi = 0$) is a trivial fixed point. By definition $0 \leq \xi \leq \frac{1}{2}$, and from Eq. 11 we see that $0 \leq J(\xi) \leq \frac{1}{2}$. We claim that starting with $\xi = 1/2$ and iterating the process $\xi \rightarrow J(\xi)$ leads to a non-trivial fixed point satisfying:

$$\xi(k_z = Q/2) = \frac{1}{2}.$$  

(12)
Indeed, by (8) the kernels of $T^\pm$ are positive, thus $T^\pm$ are positivity preserving linear operators: if $\xi \geq \xi'$, then $T^+\xi \geq T^+\xi'$; similarly $T^-\sqrt{1/4-\xi^2} < T^-\sqrt{1/4-\xi'^2}$, and consequently:

$$\xi \geq \xi' \implies J(\xi) \geq J(\xi').$$  \tag{13}$$

Thus starting with $\xi_0 = 1/2$, we have $J(\xi_0) \leq \xi_0$ and setting $\xi_n = J(\xi_{n-1})$, $\xi_n$ is a decreasing sequence of positive functions and thus converges to a fixed point $\xi_\infty$.

1-D approximation. Now we impose that $b_k$ (thus $\xi_k$) is non zero only in the cylinder $C$ corresponding to the gray region of Fig.1 where it depends only on $k_z$: $C = \{ k : k_x^2 + k_y^2 \leq r^2 = 1 - (1 - \epsilon)^2 \approx 2\epsilon, 0 \leq k_z \leq Q \}$. As we shall see below, $b_k$ differs from zero only in the neighborhood of the top disk of $\mathcal{F}_\xi$ (and its symmetric for $\mathcal{F}_{-\xi}$). In any case, these restrictions always provides an upper bound for the energy of the SDW.

First, for the second term of Eq.9, we have:

$$(a^2, T^-b^2) = (b^2, T^-a^2) = (b^2, T^-1) - (b^2, T^-b^2) \tag{14}$$

From Eq.8

$$T^+ - 1 = v_F(k) - v_F(\bar{k})$$

where $v_F$ is the potential induced by the truncated sphere. In the spherical case, the potential of the unit sphere is given by:

$$v(k) = 2\pi + \frac{1 - k^2}{k} \ln \left|1 - k\right|$$

In this case, for $k$ close to 1 ($k$ and $\bar{k}$ are close and near the unit sphere and $k_z = 2 - k_z$), $v(k) - v(\bar{k}) \approx -4\pi(1 - k) \log\left(\frac{1 - k}{k}\right)$. This singular behavior is associated to the discontinuity of the density (in k-space). An analytic solution is provided for the truncated sphere [13]. This solution has the same behavior except that 1 - $k$ has to be replaced by the distance of $k$ to the discontinuity of the density, i.e. the top disk of $\mathcal{F}_\xi$:

$$(T^-1)(k) \approx -4\pi(\nu/2 - k_z) \log \left(\frac{\nu/2 - k_z}{2}\right) \tag{15}$$

provided that $|\nu/2 - k_z| \ll 1$. For $h > 0$, Eq.[15] is still valid [13] except in a small neighborhood of the edge of the top disk. In the following we neglect this effect and apply Eq.[15] also for $h > 0$.

Using the scaled distance $x = (\nu/2 - k_z)/r$,

$$2k + T^- - 1 = 2\pi r(\nu x - 2x \log(x)) \tag{16}$$

and integrating over $q = (k_x, k_y)$, Eq.[9] becomes:

$$\Delta E_{\text{sdw}}^F = 4\pi a \nu r^4 \int_{r_s} \delta E_{\text{sdw}}^F \tag{17}$$

$$\delta E_{\text{sdw}}^F = 2\pi(\nu x - 2x \log(x), \nu a^2) - (T^- b^2, b^2) - (T^+\xi, \xi) \tag{18}$$

where the scalar product is now $(f, g) = \int_{x > 0} dx f(x)g(x)$, and $T^\pm$ become in terms of $x$:

$$(T^\pm f)(x) = \pi \int_0^{1/r} dx' (G(x - x') \pm G(x + x')) f(x') \tag{19}$$

$$G(x) = \frac{1}{\pi^2 x^2} \int_{q^2 + q'^2 < r^2} dq dq' = 1 \left|\frac{1}{q'^2 - (q - q')^2} \right| \tag{20}$$

In fact, for small $r_s$, the term $(T^- b^2, b^2)$ may be neglected in Eq.[18] [13]. In any case, since $T^-$ is a positive operator, we get an upper bound for the energy and the variation of the resulting upper bound leads to $\xi = J\xi$ where $J$ is now an operator on the positive functions on $\mathbb{R}^+$:

$$J(\xi) = \frac{1}{2} \sqrt{(x^2 \gamma \log(x))^2 + (T^+\xi)^2} \tag{22}$$

As above, the fixed point of Eq.[22] can be easily found by iteration.

Thereafter, for fixed $r_s$ the total energy variation $\Delta E(\epsilon, h) = \Delta E_{\text{FG}}^F(\epsilon, h) + \Delta E_{\text{sdw}}^F(\epsilon)$ is computed and optimized with respect to $\epsilon$. For $r_s = 3$ about 20 iterations of the operator $J$ are required and about 100 iterations for $r_s = 0.01$ (see ▲ symbols in Fig.3). In the next paragraph, we give a solution for $\xi$ at small $r_s$ and deduce the scaling of $\Delta E$ from it.

Analytic solution for small $r_s$. For small $r_s$, $\gamma$ is large and Eq.[22] can be solved approximately [13]:

$$\xi(x) \approx \frac{1}{2} \frac{\sqrt{x^2 \gamma} + 1}{\sqrt{x^2 \gamma} - 1} \cos \left(\frac{1}{2} \sqrt{x^2 \gamma} \arcsinh \left(\frac{x}{x_0}\right)\right) \tag{23}$$

$$x_0 = 2 \exp\left(-\frac{\pi}{2\sqrt{2}} \sqrt{\gamma} - \frac{1}{2}\right) \tag{24}$$

![FIG. 3: Renormalized energy $\Delta E_{\text{sdw}}^F / r_s^3$ as a function of the density. The dashed-dotted line stands for the analytical solution: $\Delta E_{\text{sdw}}^F / r_s^3 = -0.115$. ▲ stand for the SDW simulations. Others symbols stand HF energies (see Fig.5 of [6]).](image-url)
computations of the jellium [6, 7] we have considered a
in Eqs. 27 and 28 behave as
This can be verified on the figure: the next corrections
F energy gain to deeply rely on the precise shape of
r larger (thus
α parameter
∆r ≈ −E
s
ϵ/ϵ
s
γ/√r
energy
r
s
3
decimal
when
h
r
s
3
decades
r
s
3 can be mostly
k-points
used
b
k
= 0).
Direct numerical simulations of the
SDW in this high density region will require a significant
increase of k-points by several order of magnitudes.

Conclusion. Considering the ground state of the jellium
in the Hartree-Fock approximation, we quantified the
energy of the SDW suggested by Overhauser. Furthermore,
we prove that a modification of the truncated Fermi sphere
becomes crucial, and even the simulations with 128
k-points used in [6] are insufficient to resolve the expected
SDW amplitudes leading to the standard Fermi gas ground state
(α = 0 and b
k
= 0). Direct numerical simulations of the
SDW in this high density region will require a significant
increase of k-points by several order of magnitudes.

Our results readily extends to a polarized model: in
Eq. [7] we have to take into account the direct potential
which appears with a factor 1/Q2 and thus is negligible
at small rs (of order ϵr).

In order to obtain the energy of jellium, the results
of Fig. 4 must be multiplied by the number of SDW. For
simple periodic models considered in previous works, this
factor varies from 2 (hexa) up to 12 (bcc). At very small
rs, the perturbation of the SDW is localized in tiny re-
regions which do not interact, thus, one may suppose that
we can have many of them distributed around the Fermi
sphere giving rise to a quasi-periodic behavior of the density.

for
2π√2(γ' − γ) = √7(π2 + 4), leading to the asymptotic
behavior of ∆E
Fslow:

\[ \Delta E_{\text{Fslow}}(\epsilon) \leq -C \frac{2\pi^2 a V}{r_s^2} \epsilon^2 \exp \left( -\frac{\pi}{\sqrt{2} \gamma} \right) \] (25)

with \( C = 8 e^{-3/2 - \pi^2/8} \).

Now Eq. 4 and Eq. 25 provide the behavior of \( \Delta E(\epsilon, h) \):

\[ \Delta E = \Delta E_{\text{Fslow}} + \Delta E_{\text{FG}} \]
\[ = \frac{2\pi^2 a V \gamma^2}{r_s} \left( c_0 - C \exp \left( -\frac{\pi}{\sqrt{2} \gamma} \right) \right) \] (26)

The minimum energy is at \( \epsilon = \epsilon_0 (1 + O(\sqrt{r_s})) \):

\[ \Delta E \approx -\frac{\pi a K}{r_s^2} \epsilon^3 \] (27)
\[ \epsilon_0 = \frac{2C}{3a} e^{-\pi^2/4 - \pi(\gamma^2/2)} \approx 0.0294 e^{7.714/\sqrt{\gamma}} \] (28)

where \( \gamma_0 = a K / (a V \pi r_s) \). Eq. 27 shows that at small rs,
\( \Delta E r^2 / \epsilon^3 \) goes to a constant. Fig. 3 shows the numerical
results for the scaled energy at \( h = 1/2 \) (● symbols).
This scaled energy is of order of 0.1 over a wide range of
r. On the other hand, while \( \epsilon_0 \), Eq. 25 varies over
decades when \( r_s \) decreases, Fig. 3 shows that the ratio
\( \epsilon / \epsilon_0 \) is a slowly varying function. The analytical result is
supposed to be relevant for large \( \gamma \) that is for \( \sqrt{r_s} \gg 1 \).

Influence of \( h \). The dependency in \( h \) is through the
parameter \( \alpha \), see Eq. 4. Fig. 5 shows the effect of \( h \) on \( \epsilon \)
and \( \Delta E \) obtained numerically. For small \( r_s \), at \( h = 1/2 \)
(thus \( \alpha = 1/6 \)), the energy is actually 16 times larger
than in the Overhauser model (\( h = 0, \alpha = 2/3 \)). At
larger \( r_s \), this ratio can be significantly increased, e.g.
it is about 200 for \( r_s = 5 \); in this region we expect the
energy gain to deeply rely on the precise shape of \( F \).

Comparison with HF simulations. In previous HF
computations of the jellium [6, 7] we have considered a
discretized Fermi sphere of 643, 963 and 1283 values of
\( k \). This corresponds to 32, 48 and 64 equally distributed values of
\( k \) in the interval (0, 1). For \( r_s < 5 \) evidence for SDW ground states have been found [6]. In Figs 3 and
4 we show the corresponding energy gain per number of
SDW (2 for hexa up to 12 for bcc). The larger energy
gain of the HF simulations for \( r_s \geq 3 \) can be mostly
attributed to a smoother and better optimized shape, com-
pared to the simple cylinder used in the analytical SDW;
other assumptions such as the 1-dimensional approxima-
decrease the energy further by a factor of 2 −3. For
\( r_s < 3 \), the discretization of the Fermi sphere becomes
crucial, and even the simulations with 128
k-points used
in [6] are insufficient to resolve the expected SDW am-
plitudes leading to the standard Fermi gas ground state
(\( \epsilon = 0 \) and \( b_k = 0 \)). Direct numerical simulations of the
SDW in this high density region will require a significant
increase of k-points by several order of magnitudes.

FIG. 4: Scaled parameter \( \epsilon / \epsilon_0 \) as a function of the density. \( \epsilon_0 \)
is the value of Eq. 25 for \( h = 1/2 \). The black circles stands for the
present work, while other symbols stand for HF results [6].

FIG. 5: Influence of \( h \) on the energy gain versus \( r_s \): (●) energy and (○) \( \epsilon \) ratios.
[1] S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano, Phys. Rev. Lett. 105, 086403 (2010).

[2] A. W. Overhauser, Phys. Rev. Lett. 4, 462 (1960); Phys. Rev. 128, 1437 (1962).

[3] G. F. Giuliani and G. Vignale, Quantum Theory of the Electron Liquid, Cambridge University Press, Cambridge (2005).

[4] S. Zhang and D. M. Ceperley, Phys. Rev. Lett. 100, 236404 (2008). arXiv:0712.1194 (2007).

[5] F. G. Eich, S. Kurth, C. R. Proetto, S. Sharma, and E. K. U. Gross, Phys. Rev B 81, 024430 (2010).

[6] L. Baguet, F. Delyon, B. Bernu, and M. Holzmann, Phys. Rev. Lett. 111, 166402 (2013), Phys. Rev. B, 90, 165131 (2014)

[7] L. Baguet, PHD thesis, (2014), https://tel.archives-ouvertes.fr/tel-01127918

[8] B. Bernu, F. Delyon, M. Holzmann and L. Baguet, Phys. Rev. B 84, 115115 (2011); cond-mat/0810.3559.

[9] apart from [10], but this estimate is overruled by the present work.

[10] B. Bernu, F. Delyon, M. Duneau, and M. Holzmann, Phys. Rev. B 78, 245110 (2008); cond-mat/0810.3559.

[11] For given $\epsilon$ and $0 \leq h \leq 1$, the radius of truncated sphere satisfies $R^3 \left( 4 + 3\epsilon^2(1 - 2h) + \epsilon^3(1 - 3h) \right) = 4$.

[12] One easily checks afterwards that the optimal energy is obtained for $b_k$’s with a constant arbitrary phase.

[13] For detailed demonstrations, see http://www.lptmc.jussieu.fr/lptmcdata/3DEG/SDW/