Thomas-Fermi approximation to pairing in finite Fermi systems. The weak coupling regime

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I. INTRODUCTION

Semiclassical approaches to finite Fermi systems provide a very efficient way of extracting the average behaviour of relevant physical quantities which characterize such systems. The most well known example is the celebrated Droplet Model and its extensions developed by Myers and Swiatecki which describe nicely the average behaviour of the nuclear masses [1]. Semiclassical techniques have also been applied to study the average behaviour of other properties such as inertias [2], charge radii [3], one- and two-body matrix elements[4], etc. Our aim here is to present a new Thomas-Fermi (TF) theory, i.e. the $\hbar \to 0$ limit, for describing the average trends of the effect of pairing correlations in finite Fermi systems. Semiclassical approaches to the pairing problem can be of interest in scenarios like, e.g., cold atomic gases where the huge number of particles makes the full quantal calculation numerically very complicated. Also these calculations are useful if one is only interested in the average behaviour of the pairing gap, as is the case of the pairing term in the nuclear mass formula. The Local Density Approximation (LDA) is the standard semiclassical technique for dealing with the average behaviour of the pairing which was developed by Schuck and collaborators more than twenty years ago [10]. In LDA one considers the BCS equations in

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infinite homogeneuous matter and replaces the Fermi momentum k_F by its local version in terms of the density. The validity of LDA applied to the pairing problem is restricted on one hand to situations where the local Fermi wavelength $2\pi/k_F(\mathbf{R})$ is small as compared with the distance where the mean field potential varies appreciably. In the case of a harmonic oscillator potential $V(\mathbf{R}) = m\omega^2 R^2/2$ this distance is the so-called oscillator length defined as $l = \sqrt{\hbar/m\omega}$. On the other hand, a second length scale introduced by pairing is the coherence length ξ which measures the extension of the Cooper pairs. The validity of LDA in the pairing case also implies that the coherence length be smaller than the oscillator legth, i.e. $\xi/l < 1$, which is usually equivalent to the condition $\Delta/\hbar\omega > 1$, where Δ is the gap in the single-particle spectrum. The condition $\xi/l < 1$ is always violated in the outer tail of the surface because the LDA coherence length behaves as $\xi \sim \Delta^{-1}$ and the gap vanishes in this region. In spite of these deficiences, integrated quantities as pairing energies may be quite accurate when considered on average [10].

In this contribution we present a novel TF theory for pairing which improves the LDA. This theory can be applied in the weak pairing regime where the chemical potential μ and the Fermi energy ε_F have similar values and $\Delta/\mu << 1$. This TF theory works, for the average, in the region $\Delta < \hbar\omega$, where LDA generally fails.

An important point that will be discussed in this contribution is the possible quenching of the pairing gap when approaching the drip line. This fact is well documented in the recent nuclear physics literature [5–9] and we will see, using some examples, that this effect is a general feature when superfluid (superconducting) fermions come in a finite confining potential to an overflow situation.

The contribution is organized as follows. The basic theory is presented in the second section. The main results are discussed in the third section. Our conclusions are laid out in the last section.

II. BASIC THEORY

It is well known that in the Hartree-Fock-Bogoliubov theory single-particle density matrix and the pairing tensor or anomalous density matrix are simultaneously diagonalized by the so-called canonical or natural basis, $|n_c\rangle$ [11]. As far as in this work we are only interested

in the weak coupling limit where the gap is small as compared with the Fermi energy, i.e. $\Delta/\mu < 1$, one can replace with only small error the canonical basis by the basis of the normal, non-superfluid mean field (HF) Hamiltonian. In this situation the gap equation reduces to its BCS approximation and can be written as

$$\Delta_n = -\sum_{n'} V_{nn'} \frac{\Delta_{n'}}{2E_{n'}}, \tag{1}$$

where $V_{nn'} = \langle n\bar{n}|v|n'\bar{n}'\rangle$ is the matrix element of the interaction with $|\bar{n}\rangle$ the time reversed state of $|n\rangle$ and $E_n = [(\epsilon_n - \mu)^2 + \Delta_n^2]^{1/2}$ the quasi-particle energies, with ϵ_n the diagonal elements of the normal mean field Hamiltonian [11] written in the basis of the standard mean field hamiltonian, that is $H|n\rangle = \epsilon_n|n\rangle$.

At equilibrium and for time reversal invariant systems canonical conjugation and time reversal operation are related by $\langle\mathbf{r}|\bar{n}\rangle = \langle n|\mathbf{r}\rangle \Rightarrow \langle\mathbf{r}_1\mathbf{r}_2|n\bar{n}\rangle = \langle\mathbf{r}_1|\hat{\rho}_n|\mathbf{r}_2\rangle$, where $\hat{\rho}_n = |n\rangle\langle n|$ is the density matrix corresponding to the state $|n\rangle$. Therefore the pairing matrix element can be writeen as:

$$V_{nn'} = \langle n\bar{n}|v|n'\bar{n}'\rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}'_1 d\mathbf{r}'_2 \langle\mathbf{r}'_1|\hat{\rho}_n|\mathbf{r}_1\rangle\langle\mathbf{r}_1\mathbf{r}_2|v|\mathbf{r}'_1\mathbf{r}'_2\rangle\langle\mathbf{r}'_2|\hat{\rho}_n|\mathbf{r}_2\rangle. \tag{2}$$

The density matrix $\hat{\rho}_n$ fulfills the Schödinger equation

$$(H - \epsilon_n)\hat{\rho}_n = 0, \tag{3}$$

therefore we can write $\Delta_n = Tr[\hat{\Delta}\hat{\rho}_n]$ and $\epsilon_n = Tr[H\hat{\rho}_n]$ and consequently the state dependence of the gap equation (1) is fully expressed through the density matrix $\hat{\rho}_n$.

Performing the Wigner transform (WT) of Eq.(3) and taking into account that the WT of the product of two single-particle operators $\hat{A}$ and $\hat{B}$ equals, to lowest order in $\hbar$, the c-number product of the corresponding WT's, i.e. $A(\mathbf{R}, \mathbf{p})B(\mathbf{R}, \mathbf{p})$, one easily obtains the $\hbar \to 0$ limit of Eq.(3) [11]

$$(H_{cl.} - \epsilon)f_\epsilon(\mathbf{R}, \mathbf{p}) = 0, \tag{4}$$

where $H_{cl.} = \frac{p^2}{2m^*(\mathbf{R})} + V(\mathbf{R})$ is the classical Hamiltonian which contains a local mean field potential $V(\mathbf{R})$ and a position dependent effective mass $m^*(\mathbf{R})$ and $f_\epsilon(\mathbf{R}, \mathbf{p})$ is the Wigner transform of $\hat{\rho}_n$. Equation (4) has to be read in the sense of distributions. Taking into account that $x\delta(x) = 0$ one obtains the normalized distribution function

$$f_E(\mathbf{R}, \mathbf{p}) = \frac{1}{g^{TF}(E)}\delta(E - H_{cl.}) + O(\hbar^2), \tag{5}$$

which corresponds to the Thomas-Fermi (TF) approximation of the normalized on-shell or spectral density matrix [4]. Its norm is equal to the level density (without spin-isospin degeneracy):

$$g^{TF}(E) = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{R} d\mathbf{p} \, \delta(E - H_{cl.}).$$ (6)

The semiclassical pairing matrix element can then be written as [4]:

$$V(E, E') = \int \frac{d\mathbf{R} d\mathbf{p}}{(2\pi\hbar)^3} \int \frac{d\mathbf{R}' d\mathbf{p}'}{(2\pi\hbar)^3} f_E(\mathbf{R}, \mathbf{p}) f_{E'}(\mathbf{R}', \mathbf{p}') v(\mathbf{R}, \mathbf{p}; \mathbf{R}', \mathbf{p}'),$$ (7)

where $v(\mathbf{R}, \mathbf{p}; \mathbf{R}', \mathbf{p}')$ is the double WT of $< \mathbf{r_1 r_2}|v|\mathbf{r_1' r_2'} >$. For a local translationally invariant force this matrix element reduces to $v(\mathbf{R}, \mathbf{p}; \mathbf{R}', \mathbf{p}') = \delta(\mathbf{R} - \mathbf{R}') v(\mathbf{p} - \mathbf{p}')$ with $v(\mathbf{p} - \mathbf{p}')$ the Fourier transform of the force $v(\mathbf{r} - \mathbf{r}')$ in coordinate space.

The gap equation in the TF approximation is obtained by replacing in (1) $\hat{\rho}_n$ and $V_{nn'}$ by their corresponding semiclassical counterparts Eqs. (5) and (7) respectively. In this way the TF gap equation reads

$$\Delta(E) = \int_0^\infty dE' g^{TF}(E') V(E, E') \frac{\Delta(E')}{2\sqrt{(E' - \mu)^2 + \Delta^2(E')}},$$ (8)

Eqs.(8)-(7) can readily be solved for a given mean field and the chemical potential is fixed by the usual particle number condition.

III.   RESULTS

As a realistic application of our TF theory we analyze the semiclassical pairing gaps as a function of mass number along the tin isotopic chain from ^{100}Sn to ^{132}Sn. To this end we use the D1S Gogny force [12] for both, mean field and pairing fields. The main ingredients for solving the semiclassical pairing equation (8) are the on-shell density matrix $f_E(\mathbf{R}, \mathbf{p})$ (5), which depends on the classical Hamiltonian H_{cl} that is determined by the effective mass $m^*(\mathbf{R})$ and the mean field $V(\mathbf{R})$. These two quantities, namely $m^*(\mathbf{R})$ and $V(\mathbf{R})$, are obtained through the Extended Thomas-Fermi (ETF) theory for finite-range non-relativistic interactions [13, 14]. Using these quantities as input, one obtains the level density (6) and the pairing matrix element (7) which allow to solve the gap equation (8) in our TF approximation. As explained in Refs. [14, 15], the ETF energy density functional can be transformed, inspired by the Kohn-Sham scheme, into a quantal functional from where the
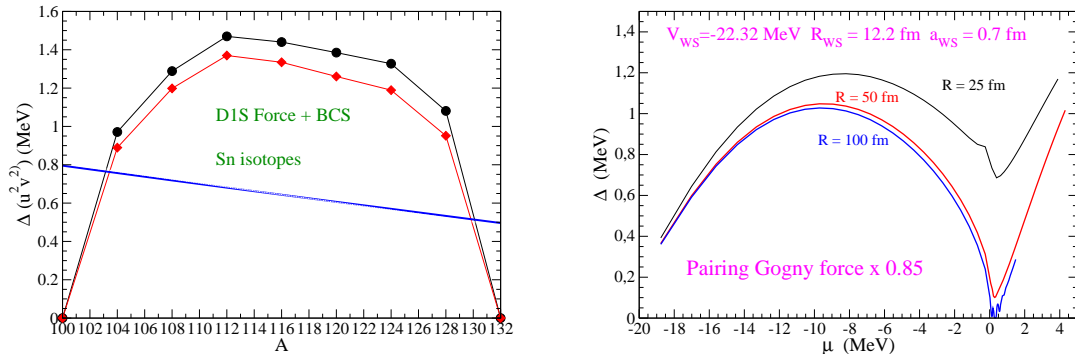
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FIG. 1: Left: Average pairing gap along the Sn isotopic chain. See text for details. Right: Average TF gaps at the Fermi energy as a function of the chemical potential in a WS potential computed in a box of radius R=25, 50, and 100 fm.

quantal average gaps are obtained. It should be noted that within this approximation the quantal functional associated to a finite- range effective interaction becomes local [14, 15]. The quantal pairing gaps averaged with u^2v^2 are depicted by circles in the left panel of Fig. 1 and show the typical arch structure. In the same panel we also display the semiclassical TF gap at the Fermi energy by a thick solid line. We see that in this case the quantal arch structure completely disappears, as expected due the absence of shell effects in this case, and that the TF gaps decrease smoothly when the neutron number increases. As it has been discussed in Ref. [16], quantal effects, i.e. the arch structure over the shell, can be almost recovered by introducing some additional quantal fluctuations in the level density and retaining the TF pairing matrix elements (7) in the gap equation (8). The average gaps obtained in these conditions are displayed by diamonds in the left panel of Figure 2. We see that the arch structure for the tin isotopic chain is recovered and that the quantal gaps are predicted quite well in this way.

An important feature of the average TF gaps is that they show a downward trend with increasing neutron number along a given isotopic chain as it can be appreciated in the left panel of Fig. 1. To investigate the behaviour of the TF gap at the Fermi energy approaching the drip line, we show in the right panel of Fig. 1 the TF gap as a function of the chemical potential employing a Woods-Saxon potential as mean field [17]. From this panel it can be seen that in the TF limit the gap vanishes just at the drip line when the chemical potential
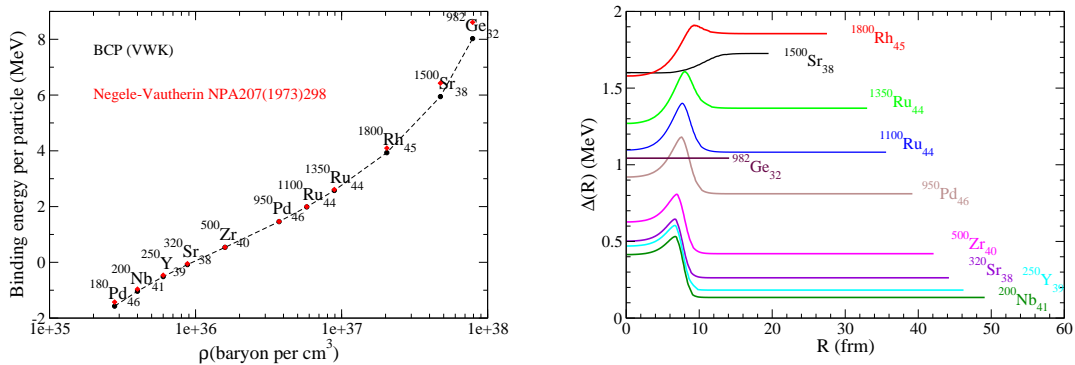
FIG. 2: Left: Energy per baryon as a function of the average density in different WS cells corresponding to the inner crust of neutron stars. Right: Radial dependence of TF gap in the analyzed WS cells. End points indicate radius of WS cells.

equals the depth of the single-particle potential. Actually we put the Woods Saxon potential in a large external container with radius R what can simulate a Wigner-Seitz (WS) cell as relevant in the inner crust of neutron stars, see below. We see that the gap becomes more and more suppressed at the edge of the Woods-Saxon potential for increasing values of the cell radius. Continuing filling the cell with a neutron gas, the gaps raise again. This quenching of the gap when approaching the drip line has also been studied by Hamamoto [5] analyzing the effective gap in weakly bound neutron levels in spherical and deformed nuclei, finding that the presence of a $s_{1/2}$ component in the wavefunction of these levels strongly reduces the effective gap. Other gap components with $l \neq 0$ show a less decreasing tendency near the drip line probably because of the centrifugal barrier which keeps the wave functions localised. This could mask the behaviour of the state dependent gaps in real nuclei near the neutron drip line.

As mentioned already, another scenario where the quenching of the neutron gap appears is near the neutron drip line in the inner crust of neutron stars. This region is a crystal of nuclei embedded in a gas of free neutrons and electrons. The inner crust was described by Negele and Vautherin [18] at HF level by means of the energy density functional method together with a spherical WS approach to deal with the crystal structure in an approximated way. The WS cell is electrically neutral and the ground state of the system of neutrons, protons and electrons is reached when they are in β-equilibrium. We have performed a

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similar calculation but at TF level and using the BCP energy density functional [19]. This functional consists of a bulk part provided by a microscopic calculation complemented by a phenomenological surface term. This functional with only four adjustable parameters reproduces nuclear binding energies and charge radii of finite nuclei with the same quality as obtained with the most performant effective forces. The ground state energy per baryon obtained in this way for average densities in the WS cells ranging from 2.79×10^{-4} to 7.89×10^{-2} fm^{-3} are displayed in the left panel of Fig. 2 (black dots) in comparison with the Negele-Vautherin results (red diamonds) finding an excellent agreement between both calculations. Although pairing correlations in the inner crust of neutron stars are mainly driven by the free neutron gas, they have, however, a noticeable influence on the composition and pairing properties of the nuclear cluster inside the WS cell [7]. On top of this TF calculation in the inner crust, we have also performed a TF pairing calculation in the studied WS cells. To this end, we have used the Gogny D1S force renormalized by a factor 0.85 to take into account that in the BCP functional the effective mass equals the physical one. A specially relevant quantity in this context is the radial dependence of the pairing gap $\Delta(\mathbf{R})$ which is obtained from the WT of the average quantal gap $\Delta_{av} = Tr[\hat{\Delta}\hat{\kappa}]/Tr[\hat{\kappa}]$ [20] which reads:

$$\Delta(\mathbf{R}) = \frac{1}{\kappa(\mathbf{R})} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \Delta(\mathbf{R}, \mathbf{p})\kappa(\mathbf{R}, \mathbf{p}) \tag{9}$$

where $\kappa(\mathbf{R}, \mathbf{p}) = \int dE g^{TF}(E)\kappa(E)f_E(\mathbf{R}, \mathbf{p})$ and $\Delta(\mathbf{R}, \mathbf{p}) = -\int \frac{d\mathbf{p}'}{(2\pi\hbar)^3}\upsilon(\mathbf{p} - \mathbf{p}')\kappa(\mathbf{R}, \mathbf{p}')$,

We see in the right panel of Fig. 2 that $\Delta(\mathbf{R})$ takes a constant value in the outer part of the WS cell which corresponds to the gap of the free neutron gas [9]. The predicted behaviour for $\Delta(\mathbf{R})$ are in qualitative agreement with previous calculations [6–9]. The nuclear cluster inside the WS cell disappears when the homogeneous phase is reached at an average density of about 0.08 fm^{-3} (^{982}Ge$_{32}$). In this case the gap in the cell is practically the gap obtained in pure neutron matter at the same density. The density of the free neutron gas diminishes in approaching to drip configurations. In this situation the gap is strongly reduced not only in the gas but also inside of the nuclear cluster (^{200}Nb$_{41}$) and it even may disappear completely in the nucleus when the drip line is reached (see right panel of Fig. 1). Therefore, locally the TF $\Delta(\mathbf{R})$'s are qualitatively different from what LDA would predict.

Conclusions and Outlook

We have presented a TF theory for pairing in finite Fermi systems for weak coupling situations where $\Delta/\varepsilon_F << 1$. This TF theory differs from the usual LDA. This essentially stems from the fact that we approximate the gap equation in configuration space and, thus, keep the size dependence of the matrix elements of the pairing force. This is not the case in LDA where the matrix elements of the force are always evaluated in plane wave basis. This semiclassical approach to pairing is only based on the usual validity criterion of Thomas-Fermi theory, namely that the Fermi wave length is smaller than the oscillator length. At no point the LDA condition that the coherence length must be smaller than the oscillator length enters the theory. Thus, the present TF approach yields for all pairing quantities the same quality as TF theory does for quantities in the normal fluid state. An interesting feature of our study is that the average gap breaks down going to the drip line. This unexpected result is confirmed by quantal calculations, though strongly masked by shell fluctuations. For systems with large numbers of particles the fluctuations should die out and, thus, the semiclassical behaviour prevail. Indeed preliminary results in a slab configuration show good agreement between quantal and TF gaps around the drip region. We also investigated in slab geometry the inverse scenario where the external potential gets in the upper part suddenly strongly constricted rather than widened. Very preliminary results show that the gaps now become much enhanced where before they were suppressed. Putting such kind of slabs into a series could create a macroscopic system with strongly enhanced pairing properties. More studies of this kind are under way.

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