SEMiclassical description of average Pairing Properties in Nuclei

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Abstract

I. Abstract

We present a new semiclassical theory for describing pairing in finite Fermi systems. It is based on taking the $\hbar \to 0$, i.e. Thomas-Fermi, limit of the gap equation written in the basis of the mean field (weak coupling). In addition to the position dependence of the Fermi momentum, the size dependence of the matrix elements of the pairing force is also taken into account in this theory. An example typical for the nuclear situation shows the improvement of this new approach over the standard Local Density Approximation. We also show that if in this approach some shell fluctuations are introduced in the level density, the arch structure displayed by the quantal gaps along isotopic chains is almost recovered. We also point out that in heavy drip line nuclei pairing is strongly reduced.

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II. INTRODUCTION

Average properties in nuclei give very valuable information about salient features of nuclear physics. The most well known example is the celebrated Droplet Model and its extensions developed by Myers and Świątecki [1]. However, not only the average of binding energies is of interest. There are other properties like inertias [2, 3], one- and two-body matrix elements [4], etc. whose average behaviour is also of interest and has been studied in the past. Our aim here is to present a new semiclassical approach to nuclear pairing based on the Thomas-Fermi (TF) theory, i.e. in the $\hbar \to 0$ limit, to study the smooth behaviour of the pairing properties. Semiclassical approaches to the pairing problem of Finite Fermi systems may be helpful in cases where the quantal fluctuations are weak or if only the average behaviour is of interest.

The standard semiclassical limit to pairing is the well known Local Density Approximation (LDA) [5]. It consists in considering the BCS equations in infinite homogeneous matter and replace the Fermi momentum $k_F$ by its local version in terms of the density. LDA is valid in situations where the local Fermi wavelength $2\pi/k_F(R)$ is small compared with the distance over which the mean field potential varies appreciably, that in the case of a harmonic oscillator (HO) potential $V(R) = m\omega^2R^2/2$ is the so-called oscillator length $l = \sqrt{\hbar/m\omega}$. Pairing introduces a second length scale that is the coherence length $\xi$ which gives the extension of the Cooper pairs. For LDA to be valid in the pairing case, also the condition $\xi/l << 1$ must be fulfilled. This condition is usually equivalent to $\Delta/\hbar\omega > 1$, where $\Delta$ is the gap in the single-particle spectrum. However, since in LDA $\xi \sim \Delta^{-1}$, there is a region in the tail of the surface where the condition $\xi/l << 1$ is violated because the gap vanishes in this region. In spite of these failures, integrated quantities as pairing energies may be quite accurate when considered in an average [5].

We present here a semiclassical theory for pairing which improves the LDA. This theory shall be applicable in the weak pairing regime where $\mu \sim \varepsilon_F$ with $\mu$ the chemical potential and $\varepsilon_F$ the Fermi energy, and, therefore $\Delta/\mu << 1$. This TF theory works, for the average, in the region $\Delta < \hbar\omega$, where in general LDA breaks down. Preliminary applications of our theory has been made in [2, 6].

The contribution is organized as follows. The basic theory is sketched in the second section. Some results are presented in the third section. Our conclusions are given in the...
III. BASIC THEORY

In the Hartree-Fock-Bogoliubov theory the so-called canonical or natural basis, \(|n_c⟩\), diagonalizes simultaneously the single-particle density matrix \(\hat{\rho}\) and the pairing tensor (anomalous density) matrix \(\hat{\kappa}\):

\[
\hat{\rho}|n_c⟩ = v_n^2 |n_c⟩, \quad \hat{\kappa}|n_c⟩ = u_n v_n |n_c⟩,
\]

where the eigenvalues \(v_n^2\) have the meaning of occupation numbers and the amplitudes \(u_n, v_n\), normalised as \(u_n^2 + v_n^2 = 1\), are analogous to the ones also used in BCS theory. In the canonical basis the gap equation has the following form:

\[
\Delta_{n_c} = -\sum_{n_c'} V_{n_c,n_c'} \frac{\Delta_{n_c'}}{2E_{n_c'}},
\]

where \(V_{n_c,n_c'} = \langle n_c\bar{n}_c|n'_c\bar{n}_c'⟩\) is the matrix element of the pairing interaction with \(|\bar{n}_c⟩\) the time reversed state of \(|n_c⟩\) and \(E_{n_c} = [(\epsilon_{n_c} - \mu)^2 + \Delta_{n_c}^2]^{1/2}\), with \(\epsilon_{n_c}\) the diagonal elements of the normal mean field Hamiltonian and \(\mu\) the chemical potential, are the eigenvalues of the HFB energy matrix.

In the weak coupling regime we have \(\Delta/\mu \ll 1\) and in this case the density and the density matrix are very little influenced by the gap. Therefore, one can replace with only little error the canonical basis by the basis of the normal, non superfluid, mean field (H.F.) Hamiltonian, that is \(H|n⟩ = \epsilon_n |n⟩\), which in terms of the density matrix \(\hat{\rho}_n = |n⟩⟨n|\) corresponding to the state \(|n⟩\) reads:

\[
(H - \epsilon_n)\hat{\rho}_n = 0.
\]

We, thus, can write \(\Delta_n = Tr[\hat{\Delta}\hat{\rho}_n]\) and \(\epsilon_n = Tr[H\hat{\rho}_n]\) and therefore the state dependence of the gap equation (2) is entirely expressed through the density matrix \(\hat{\rho}_n\).

Performing the Wigner transform (WT) of Eq.(3) and using the fact that the WT of a product of two single-particle operators is, to lowest order in \(\hbar\), equal to the product \(A(R,p)B(R,p)\) of the individual WT, we obtain for (3) in the \(\hbar \to 0\) limit:

\[
(H_{cl.} - \epsilon)f_\epsilon(R,p) = 0,
\]
where \( f_\epsilon(R, p) \) is the Wigner transform of \( \hat{\rho}_n \) and \( H_{cl.} = \frac{p^2}{2m^*(R)} + V(R) \) is the classical Hamiltonian which contains a local mean field potential \( V(R) \) and a position dependent effective mass \( m^*(R) \). Eq.\[4\] has to be understood in the sense of distributions, therefore with \( x\delta(x) = 0 \) we obtain

\[
f_E(R, p) = \frac{1}{g_{TF}(E)}\delta(E - H_{cl.}) + O(h^2),
\]

which is just the TF approximation to the normalized on-shell density matrix \[4\]. The norm is equal to the level density (without spin-isospin degeneracy):

\[
g_{TF}(E) = \frac{1}{(2\pi\hbar)^3} \int dRdp \delta(E - H_{cl.}).
\]

To derive the TF gap equation we replace \( \hat{\rho}_n \) by its semiclassical counterpart \[5\] everywhere in \[2\] obtaining

\[
\Delta(E) = \int_0^\infty dE' g_{TF}(E')V(E, E')\kappa(E')\frac{\Delta(E')}{2\sqrt{(E' - \mu)^2 + \Delta^2(E')}};
\]

where the semiclassical pairing matrix element is written as \[4\]

\[
V(E, E') = \int \frac{dRdp}{(2\pi\hbar)^3} \int \frac{dR'p'}{(2\pi\hbar)^3} f_E(R, p)f_{E'}(R', p')v(R, p; R', p'),
\]

with \( v(R, p; R', p') \) the double WT of \(<r_1r_2|v|r'_1r'_2>\) what for a local translationally invariant force yields \( v(R, p; R', p') = \delta(R - R')v(p - p') \) where \( v(p - p') \) is the Fourier transform of the force \( v(r - r') \) in coordinate space. For a density dependent zero range force, this gives \( v_0(\rho(R))\delta(R - R') \), with \( v_0(\rho) \) the density dependent pairing strength \[8\].

Eqs.\[7\]-\[8\] can be easily solved for a given mean field and the chemical potential is fixed by the usual particle number condition.

**IV. RESULTS**

First, we apply our TF theory for pairing to a model case. To this end we will use the finite-range Gogny D1S force \[9\] for the pairing channel together with a simplified mean field chosen as a simple HO potential well with constant \( \hbar\omega=8.65 \) MeV and a constant effective mass \( m^*/m = 0.8 \). This model is schematic, since it does not include the spin-orbit potential, but this simplified description contains, however, the essential physics of the problem.
FIG. 1: Left: Quantal (solid line), TF (dashed line) and LDA (double dot-dashed) line pairing gap at the Fermi energy as a function of the chemical potential in a HO potential. Right: The same but with the strength of pairing force multiplied by a factor 1.5

In the left panel of Figure 1 we display the gap at the Fermi energy as a function of the chemical potential $\mu$. In the quantal case we still perform an additional average over the substates in each major shell [10] that does not eliminate essential quantal features of the full solution, in particular the strong shell fluctuations are preserved. We see the break-down of pairing in the vicinity of closed HO shells. The dashed line represents our TF solution and the double dot-dashed curve shows the LDA values. We see that the TF approach averages the quantal values quite well while the LDA results seems to be too high. All three solutions show globally a wide bump behavior. At small values of $\mu$, the level density drops to zero and for high values of $\mu$ the matrix element vanishes, since the Gogny force is finite range and cannot scatter the particles to very high energies. In between the two limits where the gap vanishes, there is a maximum which has the same origine as the one of the gap in infinite matter as a function of $k_F$ [8]. In the right panel of Figure 1 we again show a similar study, only the intensity of the pairing force has been increased by a factor of 1.5. This increases the gap substantially and thus strongly smoothenes the shell effects of the quantal gaps. We see that in this scenario the TF approach yields a precise average whereas LDA leads to an overestimation by about 20 percent. Increasing the force still further, the shell oscillations disappear completely. We checked that in this case quantal and TF values practically coincide whereas the LDA values remain too high.

As a realistic application of our TF theory for pairing, we analyze the semiclassical pairing
FIG. 2: Left: Neutron effective mass (top) and single-particle potential (bottom) for the nucleus $^{116}$Sn. Right: Level density (top) and accumulated level density (bottom) of the nucleus $^{116}$Sn computed with fluctuations (solid line) and without (TF) (dashed line).

gaps as a function of mass number along the tin isotopic chain from $^{100}$Sn to $^{132}$Sn using the D1S Gogny force for both, mean field and pairing field. The main ingredient for solving the semiclassical pairing equation (7) is the on-shell density matrix $f_E(R, p)$ (5), which depends on the classical Hamiltonian $H_{cl}$ that is determined by the effective mass $m^*(R)$ and the mean field $V(R)$. To obtain these quantities we use the Extended Thomas-Fermi (ETF) theory for finite-range non-relativistic interactions [11, 12]. We compute $m^*(R)$ and $V(R)$ self-consistently and the corresponding semiclassical results are displayed by dashed lines in the left panel of Figure 2 in the case of the nucleus $^{116}$Sn. Using these quantities as input, one obtains the TF level density (6) and the pairing matrix element (8) which allow to solve the gap equation (7) in our TF approximation.

We can try to recover the arch structure by introducing additional quantal information. As it is known for pairing, quantal fluctuations are more important in the level density than in the pairing matrix elements. To do that we proceed as follows. As it has been explained in Refs. [12, 13], the ETF energy density functional can be transformed, inspired by the Kohn-Sham scheme, into a quantal energy density functional. It should be noted that within this approximation the functional associated to a finite-range effective interaction becomes local. The quantal $V(R)$ and $m^*(R)$ obtained in this way are also displayed by solid lines in Figure 2. We see, as expected, that the quantal oscillations are nicely averaged by the ETF solutions.
For a given nucleus, once the single-particle energy levels have been obtained, we build a fluctuating level density by taking a sum of Gaussians each one centered at a single-particle energy, with a width $\sigma = 0.5$ MeV and with a strength such that the area below the Gaussian equals the degeneracy of each energy level (spherical symmetry is assumed). This fluctuating level density $\tilde{g}(E)$ corresponding to the nucleus $^{116}$Sn is displayed in the top of the right panel of Figure 2, where we also show, for comparison, the smooth TF level density $g^{TF}(E)$. In the bottom of the same panel the accumulated level density with and without quantal fluctuations is also displayed. We solve now the gap equation (7) using the fluctuating level density $\tilde{g}(E)$ but retaining the semiclassical matrix elements. The quantal features of pairing are essentially recovered in this way. The average quantal gaps weighted with $u^2v^2$ (circles) and the ones obtained with our TF theory for pairing using the fluctuating level density (diamonds) for the tin isotopic chain as a function of the mass number are displayed in Figure 3. We see that by introducing $\tilde{g}(E)$ the quantal arch structure is recovered and that the semiclassical gaps obtained in this way reproduce quite accurately the quantal values. In the same Figure we also display the semiclassical averages of the gap computed with the smooth TF level density (solid line). We see that in this case the quantal arch structure is completely washed out and that the semiclassical average gaps show a downward tendency with increasing neutron number. This downward trend also is clearly seen if one follows the quantal results over several major shells. In order to point out more clearly the behavior of
the gap at the Fermi energy going to the drip line, we show in the right panel of the figure the behavior of the gap as a function of the chemical potential. We see that in the TF limit the gap vanishes when $\mu$ equals the depth of the single-particle potential, i.e. exactly at the drip. This should be relevant for instance for nuclei in the outer crust of neutron stars [14] or for other finite Fermi systems with a large number of particles.

Conclusions

We have presented a TF theory for pairing in finite Fermi systems for weak coupling situations where $\Delta/\varepsilon_F \ll 1$. 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 the TF 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 in 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.

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