Generic size dependences of pairing in ultrasmall systems: electronic nano-devices and atomic nuclei

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Abstract We study the average and global pairing behaviours of electronic devices, like films, wires, and grains using semiclassical methods, such as Weyl and Thomas–Fermi approximations, in the ultrasmall, i.e., quantal regime, which exhibits strong quantum fluctuations and shell effects. We discuss how these results, mostly analytic, are elaborated for average size dependencies, in order to be used in other circumstances when the fully quantal calculation become computationally too expensive. We also compare the results with latest experimental ones where possible.

1 Introduction

The discovery of superconductivity dates back to 1911 [1], when Kammerlingh–Onnes found that at very low temperature the resistivity of certain metals drops to zero. The first microscopic interpretation of these new phenomena appears in 1957 [2] thanks to the remarkable work of Bardeen, Cooper and Schrieffer (BCS). One year later, Bohr, Mottelson and Pines [3] suggested that such a theory could also be used to explain some interesting phenomena concerning the position of nuclear excited states.

This work was one brilliant example of cross contamination between different fields of research and how some phenomena are universal, i.e., independent of some specific details of the system under analysis. Atomic nuclei were the first objects where strong shell effects as a function of the particle (nucleon) number, i.e. as a function of size, have been observed, see, e.g., Refs. [4,5]. These structures have been explained since long using Hartree–Fock–Bogoliubov (HFB) or BCS theory [4,5]. On the other hand, electronic devices are usually of macroscopic scale and thus such small quantal fluctuations are not important.

In recent years, with the advent of technological procedures to fabricate nano grains, films and wires, the study of pairing in metallic nano systems has made a lot of progress [6]. In those condensed matter systems, one rather talks about the Bogoliubov de Gennes (BdG) approach to which reduces HFB for zero range pairing interactions. Also the diagonal approximation of the gap is in use in nuclear physics as well as in condensed matter systems, in the former it is called BCS because of its similarity with the BCS equations of homogeneous matter whereas for condensed matter nano systems one usually talks about the ‘Anderson’ approximation because it was P.W. Anderson who proposed this in 1959 [7]. It turns out that the BCS/Anderson approximation works reasonably well both in nuclear and metallic systems. This stems from the qualitatively similarly shaped mean field in both cases with a flat interior and a steep surface, that is a Fermi function like potential [8]. In metallic nano systems great experimental achievements have been accomplished in the last 1-2 decades, but theory has not been at rest and impressive works for the numerical solution of nano-sized superconductivity have been published in recent years [9–16]. In these references also experimental results are given when they exist together with their citations.

In this paper, our emphasis is not so much on repeating or improving the exact solutions of the HFB/BdG equations, but to study the average and generic size dependencies of pairing
in the different systems. For nuclei this size dependence has been described by the purely empirical law $12/\sqrt{A}$ see, e.g., [4, 5] where $A$ is the number of nucleons in the nucleus. This law describes the average trend reasonably well. It turns out that also in metallic nano-systems pairing becomes, on average, stronger with reduced sizes. It is one of the main objectives of this work to explain the underlying general reasons for this behaviour. The employed tools for this investigation shall be semi-classical methods, mainly based on Thomas–Fermi (TF) and Weyl approaches which is a semiclassical technique to deal with mean field potentials with hard walls [17]. We shall point out here that in a previous paper [18] we applied the Weyl approach to study in ultra-thin films the dependency of the gap on the film thickness. In the present work, we want to enlarge this investigation in ultra-thin films and also perform similar studies in other nano-devices structures such as wires and grains.

The paper is organised as follows. In Sect. 2, we will explain how one can successfully exploit TF and Weyl theories for the solution of the gap equation. In Sect. 3, we will demonstrate with generic examples like metallic films, wires, and grains the dependence of the pairing gap on changing sizes. We will present our conclusions in Sect. 4.

2 Theoretical framework

2.1 Brief review of the quantal forma

Before considering electronic devices, for completeness, in this section, let us give a compact presentation of what was accomplished previously with a semiclassical approximation of what one calls in nuclear physics the BCS method, a name which we also want to keep in this paper for brevity. This method assumes that the gap field $\Delta_{\nu,\nu'}$ has the same form as in infinite homogeneous matter acquiring the following diagonal expression

$$\Delta_{\nu\nu'} \simeq \Delta_{\nu} \delta_{\nu',\tilde{\nu}} \equiv \Delta_{\nu} \delta_{\nu',\bar{\nu}}, \quad (1)$$

where the single particle (s.p.) states, labeled by the index $\nu$, are expressed in the canonical basis, which in the weak coupling regime can be replaced by the Hartree–Fock or mean-field one. In Eq. (1) $\bar{\nu}$ is the time reversed state of $\nu$. This approximation is valid, as we will show, for situations at equilibrium and at time reversal invariance with mean field potentials that have rather steep surfaces as they are encountered for real systems as, e.g., nuclei and metallic nano-particles. On the contrary, in cold atom systems, most of the time a wide harmonic oscillator confining external potential is used invalidating completely the use of the BCS approximation [19].

So let us assume that the BCS approximation is valid. The gap equation can be written as

$$\Delta_{\nu} = -\sum_{\nu'} V_{\nu\nu'} \frac{\Delta_{\nu'}}{2E_{\nu'}} = -\sum_{\nu'} V_{\nu\nu'} \kappa_{\nu\nu'}, \quad (2)$$

where $V_{\nu\nu'} = \langle \bar{\nu} | \langle \nu | \nu' \rangle \rangle$ is the matrix element of the pairing interaction and $\kappa_{\nu_1, \nu_2} = \sum_{\nu'} \kappa_{\nu_1 \nu} \phi_\nu (\nu_1) \phi_{\bar{\nu}} (\nu_2)$ is the pairing tensor in coordinate space [4]. In this paper, for simplicity, we will restrict ourselves to spin singlet pairing, which takes care of the antisymmetrisation of the matrix elements. So in the following of this work, we will consider always systems where spin singlet pairing is largely dominant and, thus, we can henceforth disregard the spin.\footnote{Notice that in the system under consideration here spin-orbit couplings are negligible hence spin is a good quantum number.}

Furthermore,

$$E_{\nu} = \sqrt{(\epsilon_{\nu} - \mu)^2 + \Delta_{\nu}^2}, \quad (3)$$

are the usual quasi-particle energies, with $\epsilon_{\nu}$ the single particle or Hartree–Fock (HF) energies of the mean-field Hamiltonian, that is $H |\nu\rangle = \epsilon_{\nu} |\nu\rangle$. The chemical potential $\mu$ is, as usual, determined by the particle number condition

$$N = \sum_{\nu} \frac{1}{2} \left[ 1 - \frac{\epsilon_{\nu} - \mu}{E_{\nu}} \right]. \quad (4)$$

At equilibrium and for time reversal invariant systems, canonical conjugation and time reversal operations are related by

$$\hat{\rho}_\nu (r_1, r_2) = \rho_{\bar{\nu}} (r_1, r_2),$$

$$a \rho_{\nu} (r_1, r_2) = \phi_{\bar{\nu}} (r_1) \phi_{\nu} (r_2)$$

and

$$[4,5]$$

where $\kappa_{\nu_1, \nu_2}$ is the matrix element of the pairing tensor in coordinate space [4]. In this paper, for simplicity, we will restrict ourselves to spin singlet pairing, which takes care of the antisymmetrisation of the matrix elements. So in the following of this work, we will consider always systems where spin singlet pairing is largely dominant and, thus, we can henceforth disregard the spin.\footnote{Notice that in the system under consideration here spin-orbit couplings are negligible hence spin is a good quantum number.}

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by the density matrix $\hat{\rho}_\nu$. For further details see Refs. [20–23].

2.2 Semiclassical approximations

2.2.1 The Thomas–Fermi approach to the BCS problem in mean-field potentials

The Wigner transform (WT) of an operator $A$ is defined by [4]

$$A(R, p) = \int ds e^{-ip\cdot s/\hbar} \left\{ R + \frac{1}{2} s | A | \frac{1}{2} s \right\},$$

where $R = (r + r')/2$ and $s = r - r'$. Performing the WT of Eq. (7) 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 WTs, i.e., $A(R, p)B(R, p)$, one easily obtains the $\hbar$-limit of Eq. (7) as

$$(H_{\text{cl}} - \epsilon) f_\nu(R, p) = 0,$$

where $H_{\text{cl}} = \frac{p^2}{2m^*} + U(R)$ is the classical Hamiltonian which contains a local mean field potential $U(R)$ and a position dependent effective mass $m^*(R)$ and $f_\nu(R, p)$ is the WT of $\hat{\rho}_\nu$. Equation (9) has to be read in the sense of distributions. Taking into account that $\delta(\chi) = 0$, where $\delta(\chi)$ is the Dirac delta function, here with $\chi = H_{\text{cl}} - \epsilon$, one obtains for the normalised distribution function [20–24]

$$f_\nu(R, p) = \frac{1}{g^{\text{TF}}(E)} \delta(E - H_{\text{cl}}) + O(\hbar^2),$$

which corresponds to the Thomas–Fermi (TF) approximation of the normalised on-shell or spectral density matrix $\rho_\nu(r_1, r_2) \leftrightarrow f_\nu(R, p)$ [18]. Its norm is equal to the level density (without spin-isospin degeneracy)

$$g^{\text{TF}}(E) = \int \frac{dR dp}{(2\pi \hbar)^3} \delta(E - H_{\text{cl}}).$$

Corrections to those expressions in powers of $\hbar$ can be found in textbooks [4]. The semiclassical pairing matrix element can then be written as [18]

$$V(E, E') = \int \frac{dR dp}{(2\pi \hbar)^3} \int \frac{dR' dp'}{(2\pi \hbar)^3} f_\nu \times (R, p) f_\nu^*(R', p') \nu(R, p; R', p'),$$

where $\nu(R, p; R', p')$ is the double WT of $(r_1, r_2) \leftrightarrow (r'_1, r'_2)$. For a local translationally invariant force, this matrix element reduces to $\nu(R, p; R', p') = \delta(R - R') \nu(p - p')$, with $\nu(p - p')$ the Fourier transform of the force $\nu(r - r')$ in coordinate space.

The gap equation in TF approximation is obtained by replacing in Eq. 2, the matrix elements $V_{nn'}$ by their corresponding semiclassical counterparts. In this way, the TF gap equation reads

$$\Delta(E) = -\int_0^\infty dE' g^{\text{TF}}(E') V(E, E') \kappa_{E'},$$

with

$$\kappa_E = \frac{\Delta(E)}{2E_{\text{eq,p}}(E)}$$

$$E_{\text{eq,p}}(E) = \sqrt{(E - \mu)^2 + \Delta^2(E)}.$$
where $R_0$ is the border of the box and $k_E(p_x, p_y) = \sqrt{\frac{\hbar^2}{2m} (E - \frac{p_x^2 + p_y^2}{2m})} = \sqrt{\frac{p_x^2}{p_E^2} + \frac{p_y^2}{p_E^2}}$. Performing the integral over momenta one obtains the spectral density

$$\rho_E(R) = \frac{1}{4\pi^2} \frac{2m}{\hbar^2} \frac{p_E}{g(E)} \left[ 1 - j_0(2Rp_E) \right],$$

(21)

where $j_0(x) = \sin x / x$ is the zeroth-order spherical Bessel function. The density of states can be obtained by integrating the spectral density over $R$ assuming semi-infinite geometry.

$$g(E) = \frac{1}{4\pi^2} \frac{2m}{p_E} \int (1 - j_0(2Rp_E)) dR = \frac{1}{4\pi^2} \frac{2m}{p_E} V \left( 1 - \frac{\pi S}{4p_E V} \right),$$

(22)

where we have used that $\int_0^\infty \frac{\sin(qx)}{x^4} dx = \frac{\pi q}{2}$ if $q > 0$.

The pairing matrix element in Eq. (12) can be recast as

$$v(E, E') = -\frac{\psi_0}{g(E)g(E')} \frac{1}{16\pi^4} \left( \frac{2m}{\hbar^2} \right)^2 p_E p_E' \times \int dR \left( 1 - j_0(2Rp_E) \right) \left( 1 - j_0(2Rp_E') \right),$$

(23)

where we have performed the $p$ and $p'$ integrals and used the spectral density Eq. (21). By writing explicitly the spherical Bessel functions, proceeding as before to obtain the density of states, Eq. (22), and taking into account that $\int_0^\infty \frac{\sin(qx)\sin(q'y)}{x^4} dx = \frac{\pi q}{2}$ if $q' > q > 0$, one finally obtains

$$v(E, E') = -\frac{\psi_0}{g(E)g(E')} \frac{1}{16\pi^4} \left( \frac{2m}{\hbar^2} \right)^2 p_E p_E' \times \left( V - \frac{\pi S}{4p_E} - \frac{\pi S}{4p_E'} + \frac{\pi S}{4p_E p_E'} \min(p_E, p_E') \right).$$

(24)

which in the case of $E = E'$ and taking into account explicitly the density of states $g(E)$ given by Eq. (22) one can write

$$v(E) = -\frac{\psi_0}{V} \left( 1 + \frac{\pi S}{4p_E V} \right).$$

(25)

In these expressions for the density of states (22) and the pairing matrix elements (25), we have assumed that the box is filled by matter at a given momentum $p_E$, in spite that the walls of the container compress the matter. To take into account this effect and following Ref. [26], we introduce the mass volume $V_M$ and surface $S_M$, which are related to the volume and surface of the box by the relationships

$$V = V_M + \frac{3\pi}{8p_F} S_M S = S_M \rightarrow V = V_M \left( 1 + \frac{3\pi}{8p_F V_M} S_M \right),$$

(26)

where $p_F$ is the Fermi momentum of the matter in the box, but taking into account the compressional effect. Due to the particle number conservation, it is related to the Fermi momentum in homogeneous nuclear matter (i.e. in the bulk) $p_F^B$ by

$$p_F^3 V_M = p_F^B 3 V \rightarrow p_F = p_F^B \left( 1 + \frac{\pi}{8p_F^B V_M} S_M \right).$$

(27)

Now we can write the density of states and the matrix element in the box at the Fermi energy as

$$g(\mu) = \frac{1}{4\pi^2} \frac{2m}{\hbar^2} p_F^B \left( 1 + \frac{\pi S}{8p_F^B V_M} \right) \times V_M \left( 1 + \frac{3\pi}{8p_F^B V_M} \right) \left( 1 - \frac{\pi S}{4p_F^B V_M} \right)
= \frac{1}{4\pi^2} \frac{2m}{p_F^B V_M^3} \left( 1 + \frac{3\pi}{8p_F^B V_M} \right),$$

(28)

$$v_{sc}(\mu, \mu) = -\psi_0 \left( 1 + \frac{\pi S}{4p_F^B V_M} \right) \times V_M \left( 1 - \frac{3\pi}{8p_F^B V_M} \right) = -\frac{\psi_0}{V_M} \left( 1 - \frac{\pi S}{8p_F^B V_M} \right).$$

(29)

Using these expressions, we can finally write

$$g(\mu)v_{sc}(\mu, \mu) = -\psi_0 \frac{1}{4\pi^2} \frac{2m}{\hbar^2} p_F^B \left( 1 + \frac{\pi S}{8p_F^B V_M} \right)
= -\psi_0 \frac{1}{8p_F^B V_M} \left( 1 + \frac{\pi S}{8p_F^B V_M} \right),$$

(30)

which is in agreement with the results of Ref. [18] and where $p_F^B = \frac{1}{4\pi^2} \frac{2m}{\hbar^2} p_F^B$ is the density of states per unit of volume in the bulk.

3 Metallic nano-devices

In this section, we will deal with superconducting nano-systems such as thin metallic films, nano-wires, and nano-grains. As mentioned in the introduction, we are interested in the global average behaviour of these systems in order to extract eventual generic features and, also, provide easy to use analytical formulas for the average size dependences as far as possible. In an earlier publication, we have already considered thin films [18], but here we want to extend our study in various directions making use of the semiclassical Weyl approximation for mean field potentials with hard walls what seems to be a valid approximation for metallic nano-systems.

3.1 Films

Experimental work on ultra-thin lead films [27] shows an oscillatory behaviour of the transition temperature when the
film thickness in increased. This is a manifestation of the strong quantisation effect and the creation of electronics bands that vary in position with the thickness of the film [11]. Following a previous work [18], we want to show how the semiclassic method presented here is capable to grasp these features.

The films have a slab geometry with a finite thickness \( L \) limited by infinite hard walls in the transverse direction. The normalized wavefunction in this case reads

\[
\phi_{np\perp} = \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi z}{L} \right) \frac{e^{i p \perp z}}{\sqrt{S}},
\]

where \( S \) and \( L \) are the surface and thickness of the film, respectively. The single-particle wavefunctions across the film thickness are quantized with eigenvalues

\[
E_n = \frac{\hbar^2}{2m} \left( \frac{\pi}{L} n \right)^2; \quad n = 1, 2, \ldots
\]

while along the transverse direction the wavefunctions are plane waves with kinetic energy \( e_\perp = \frac{p^2}{2m} \).

Using Eq. (31) the pairing matrix element (6) can be written as

\[
\langle n p\perp \mid |n\perp p\perp \rangle = - \frac{2g_{L S}}{L S} \Theta_{np\perp} \Theta_{n'p'\perp} \frac{2}{L} \int dz \sin^2 \left( \frac{n \pi z}{L} \right) \sin^2 \left( \frac{n' \pi z}{L} \right) = \tilde{v}_0(n, n') \Theta_{np\perp} \Theta_{n'p'\perp}.
\]

Notice that the range of the pairing matrix element is bounded by the Debye frequency \( \omega_D \), which defines the window where the pairing acts

\[
\Theta_{n,p} = \Theta(\omega_D - |E_n + e_\perp - \mu|).
\]

Using this matrix element the gap equation (2) reads

\[
\Delta_{n,p\perp} = \Theta_{n,p\perp} \sum_{n',p'\perp} \tilde{v}_0(n, n') \frac{\Theta_{n',p'\perp} \Delta_{n',p'\perp}}{(E_{n'} + e_\perp - \mu)^2 + \Delta_{n',p'\perp}^2} = \Theta_{n,p\perp} \sum_{n'} \tilde{v}_0(n, n') \frac{1}{2} \int_0^\infty \frac{d^2 p'_\perp S}{(2\pi \hbar)^2} \times \frac{\Theta_{n',p'\perp} \Delta_{n',p'\perp}}{(E_{n'} + e_\perp - \mu)^2 + \Delta_{n',p'\perp}^2}.
\]

In the weak coupling regime, we assume that the gap is strongly concentrated around the Fermi energy and thus the only relevant pairing matrix elements are the diagonal ones. In this limit, we define the state dependent gap as \( \Delta_{n,p\perp} = \Delta \Theta_{n,p\perp} \), where \( \Delta \) is an average gap, which allows to write the gap equation (35) as

\[
1 = \frac{1}{L} \frac{V}{4\pi} \frac{2m}{\hbar^2} \sum_{n'} \tilde{v}_0(n', n') \frac{1}{2} \int_0^\infty de_\perp \times \frac{\Theta_{n',e_\perp} \Delta_{n',e_\perp}}{2\sqrt{(E_{n'} + e_\perp - \mu)^2 + \Delta^2}},
\]

where we have introduced the volume of the film \( V = SL \) and changed the integration variable from \( p_\perp \) to \( e_\perp \).

Now we replace each quantal matrix element \( \tilde{v}_0(n', n') \) in the pairing window by the semiclassical matrix element computed at the Fermi energy \( v_{sc}(\mu, \mu) \), see Eq. (29). Making a change of variables

\[
\xi = E_n + e_\perp - \mu,
\]

we obtain, together with the assumption \( \Delta \ll \omega_D \), the standard weak coupling expression

\[
1 = \frac{v_{sc}(\mu, \mu) V}{L} \frac{2m}{4\pi} \frac{1}{\hbar^2} \sum_{n} \Theta(\mu - E_n) \int_{-\omega_D}^{\omega_D} d\xi \frac{1}{2\sqrt{\xi^2 + \Delta^2}} = v_{sc}(\mu, \mu) g F(\mu) \ln \left( \frac{2\omega_D}{\Delta} \right),
\]

where we have introduced the quantal density of states (DOS) for a slab of thickness \( L \), which is given by

\[
g_f(\mu) = \frac{V}{L} \sum_{n} \int \frac{d^2 p_\perp}{(2\pi \hbar^2)} \delta \left( \mu - E_n - \frac{p_\perp^2}{2m} \right) = \frac{1}{L} \sum_{n} \frac{V}{4\pi} \frac{2m}{\hbar^2} \Theta(\mu - E_n).
\]

The average gap is easily extracted from Eq. (37) and reads

\[
\Delta = 2\omega_D \exp \left[ - \frac{1}{v_{sc}(\mu, \mu) g F(\mu)} \right],
\]

which clearly shows the dependence of the gap on the DOS in the weak coupling limit. The size dependence of the gap \( \Delta \) is thus contained in the corrections to the bulk values of the DOS, the pairing matrix element \( v_{sc} \) and the chemical potential \( \mu \).

The semiclassical DOS, derived from the Weyl formula for three dimensional bodies with infinite walls, and computed at the Fermi energy can be written as

\[
g_{sc}(\mu) = \frac{V_M}{4\pi^2} \frac{2m}{\hbar^2} k_F \left( 1 + \frac{\pi}{4\pi} \frac{S_M}{V_M} + \cdots \right).
\]

For the calculation of the gap (39) we need the matrix element with its size dependence. Replacing Eqs. (29) and (40) in Eq. (39), we finally get

\[
\frac{\Delta}{\Delta_B} = \exp \left[ - \frac{1}{|v_0| g_{sc}^B (1 + \frac{\pi}{4\pi} \frac{S_M}{V_M})} \right] \exp \left( \frac{1}{|v_0| g_{sc}^B} \right).
\]
to improve the results, we can replace in Eq. 41 the semiclassical DOS by the quantal one. Since the latter does not deviate violently from the mean value. For this, we have to be aware of the fact that the quantal DOS takes \( V_M \) and not \( V \) given in Ref. [11]. Notice we defined the level density per unit volume as \( \tilde{g}_F(\mu) = g_F(\mu)/V \), where \( g_F(\mu) \) is given in Eq. (38).

In order to be consistent, we then also have to renormalize the coupling constant \( v_0 \) by a factor \( 1 - \pi \eta S \sqrt{V} \). The expression using the box quantities. However, here it makes numerically not much difference to replace \( S/V \) by \( S_M/V_M \).

Performing all these modifications, we get to an equation that formally looks like Eq. 41; the only difference being \( \eta = \tilde{g}_F(\mu)/g_B^\rho \).

Due to the structure of the eigenvalues the evolution of \( g_F \) with energy is not smooth but it shows jumps and plateaus as illustrated in Fig. 1 for a slab of thickness \( L = 10 \) nm. From Fig. 1, we see that the semiclassical approximation is capable to provide a very good average description of the quantal one.

We are now in the position to calculate the pairing gap using the weak coupling limit formulas (41) with \( \eta = 1 \) (semiclassic) and \( \eta = \tilde{g}_F(\mu)/g_B^\rho \) (quantal) as done in Ref. [18]. For numerical values of Cd, Al, Sn, Pb, we take the ones given in Ref. [11].

In Fig. 2, we show the gap, normalized to its bulk value, \( \Delta_B \), for Cd for up to large values of \( L \) in order to demonstrate the correct behavior of the semiclassical values versus the quantal ones. In Fig. 3, we show the pairing gap normalized to its bulk value for Cd (upper left), Al (upper right), Sn (lower left), and Pb (lower right) using Eq. (41) with \( \eta = 1 \) and \( \eta = \tilde{g}_F(\mu)/g_B^\rho \). We see that, on the one hand, the fully quantal results of Fig. 1 in [11] are well reproduced and, on the other hand, the semiclassical formula (41) averages very well the quantal results (smooth continuous lines) in all cases.

Therefore, for films the average size behaviour is well described by the semiclassical analytic expressions (41). In conclusion, it is quite clear that the increase of the average gap with decreasing film thickness comes from the fact that the surface tension compresses the system more and more as its size decreases and, thus, \( k_F \) and consequently the DOS increases. The formulas can be applied to other systems, if needed. We next will turn to the case of nano-wires.

### 3.2 Wires

Recently several experiments have been performed on superconducting metallic nano-wires as discussed and cited in Ref. [10]. Those systems show shell effects which are much stronger than the ones of films. The goal of this section is to perform a similar analysis as done for the films in order to investigate the behaviour of the average pairing as a function of the wire radius. Introducing cylindrical coordinates \( r = (\rho, \phi, z) \), we now express the single particle electronic wavefunction as

\[
\phi_{jm\rho\phi}(r) = \frac{\sqrt{2}}{R J_{m+1}(\alpha_j m)} J_m \left( \frac{\alpha_j m \rho}{R} \right) \frac{e^{im\phi}}{\sqrt{2\pi}} e^{i\frac{\rho^2}{L}},
\]

where we have made the hypothesis of an infinite long wire with diameter \( 2R \). \( J_m(x) \) is the Bessel function of order \( m \) and \( \alpha_j m \) are its zeros. The structure of Eq. (42) arises from the particular choice of boundary conditions adopted for the system [9]. The BCS equation for the wire reads:

![Fig. 1 Comparison of quantal (solid) DOS with \( L = 10 \) nm as a function of \( E \) with the semiclassical expression (dashed). The constants for cadmium given in Ref. [11] are used](image1)

![Fig. 2 Quantal (solid) \( (\eta = \tilde{g}_F(\mu)/g_B^\rho) \) and semiclassical (dashed \( \eta = 1 \)) version of Eq. 41 for the normalised gap as a function of \( L \) for cadmium, see [11] for the constants](image2)
Fig. 3 Quantal and semiclassical gap using the weak coupling limit (41) for cadmium (upper left), aluminium (upper right), Tin (lower left), lead (lower right). We see almost perfect agreement with quantal solution of Shanenko in Fig. 1 of [11]  

\[ \Delta_{jm, p_z} = \frac{1}{\pi R^2} \Theta_{jm, p_z} \int_{j' m'} d p_z' d r' \frac{\Theta_{j' m', p_z' \Delta j' m', p_z'}}{\sqrt{(E_{j' m'} + \varepsilon_z - \mu)^2 + \Delta_{j' m', p_z'}^2}}, \quad (43) \]

where the matrix elements read for a simple contact interaction

\[ \tilde{\nu}_{jm; j'm'} = -\frac{g}{R^2} \int d p_j J_m^2 \frac{\alpha_j}{R} J_{m'}^2 \frac{\alpha_{j'}}{R}, \quad (44) \]

Following the same strategy already highlighted for the nano-films, i.e. supposing that the matrix elements are constant in the energy range defined by the Debye window, \( \Delta_{jm, p_z} = \Delta \Theta_{jm, p_z} \), we get the BCS gap equation as

\[ \Delta \Theta_{jm, p_z} = \frac{\Theta_{jm, p_z}}{\pi R^2} \int_{j' m'} L_{jm; j'm'} \int_{-\infty}^{\infty} d p_z' \frac{\Theta_{j' m', p_z'} \Delta}{\sqrt{(E_{j' m'} + \varepsilon_z - \mu)^2 + \Delta_{j' m', p_z'}^2}}. \quad (45) \]

\( \Theta_{jm, p_z} \) is a step function that defines the active pairing space around the Debye window and \( E_{jm} = \frac{h^2}{2m} \frac{\sigma^2_{jm}}{R^2} \). We now make a change off variable from momentum \( p_z \) to energy \( \varepsilon_z \), we get after some manipulation to the expression

\[ 1 = \frac{1}{\pi R^2} \int_{-\infty}^{\infty} d p_z \int_{jm} d E \delta(E - E_{jm} - \varepsilon_z) \frac{\Theta_{jm, j'm'} \Delta}{\sqrt{(E_{j' m'} + \varepsilon_z - \mu)^2 + \Delta_{j' m', p_z'}^2}} \]

In the weak coupling limit, we take the level density out of integral at peak value of the integrand, that is at \( E = 0 \). At this stage, we replace the quantal matrix element by its semiclassical expression \( \tilde{\nu}_{jm, j'm'} \rightarrow v_{se} V_M \). The expression of \( v_{se} \) is given in Eq. (29). We also make the change of integration variable \( \xi = E_{jm} + \varepsilon_z - \mu \) and we then obtain

\[ 1 = \frac{v_{se} V_M}{\pi R^2} \left( \frac{2m}{\hbar^2} \right)^{1/2} \int_{-\infty}^{\infty} d \xi \delta(E_{jm} - \xi) \frac{1}{\sqrt{\xi^2 + \Delta^2}}. \quad (47) \]

Actually, the integral over \( \varepsilon_z \) in Eq. (46) can be done without approximation, but the expression is in terms of the incomplete elliptic integral of the first kind which is not easy to handle. We have checked numerically that the approximation stays on top of the exact result besides very close to the divergency, where the exact solution becomes imaginary.

In order to further simplify Eq. (47) and thus recover a simpler expression, we write the expression of the quantal level density of the system as

\[ g(E) = \sum_{jm} \int_{-\infty}^{\infty} d R p_z \delta(E - E_{jm} - \varepsilon_z). \quad (48) \]

By performing the integral explicitly we get to

\[ g(E) = \frac{V}{\pi R^2} \sum_{jm} \left( \frac{2m}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{E - E_{jm}}} \]. \quad (49) \]

Going back to Eq. (47), we now identify the expression of the level density \( g(\mu) \) we just derived. By performing the integral in \( \xi \), we get to the final expression

\[ 1 = v_{se} g(\mu) \ln \frac{2\omega_D}{\Delta}. \quad (50) \]
As done for films, we now replace the quantal DOS with the semiclassical one. In Fig. 4, we compare the behavior of the quantal and semiclassical level density for a wire. Here we use the parameters given in Ref. [10] for Aluminium: $v_0 N(0) = 0.18; \omega_D = 32.3$ meV; $\mu_B = \frac{\hbar^2 B^2}{2m_e} = 900$ meV; the level density of the bulk is defined as $N(0) = \frac{\omega_D}{8\pi^2}$. The corresponding bulk Fermi momentum is then: $k^B_F = 4.83$ nm$^{-1}$; the bulk value of the gap: $\Delta_B = 0.25$ meV. From Fig. 4, we see that the quantal DOS fluctuates much more strongly than in the case of films. The semiclassical DOS reproduces the average behavior, but given the too strong fluctuations can not be considered as a satisfactory approximation.

As seen from Eq. (50), the DOS is an input to the gap equation and even though the semiclassical DOS perfectly averages the quantal DOS, it is not guaranteed that the solution of the gap equation using the semiclassical DOS as input also averages the fully quantal gap-solution well. In the case of the wires this is not the case, in contrast to the very satisfying solutions in the case of films. In order to improve the results, we introduce an empirical multiplicative factor

$$v_{sc}(\mu) \to v_0 g_B^B \left(1 + \frac{\pi}{4k^B_F R} \right) a(R),$$

which reads for Al case ($k^B_F = 4.83$ nm$^{-1}$)

$$a(R) = \frac{g(\mu)}{g_B^B} \simeq 1 \left(1 + \frac{\pi}{2k^B_F R} \right) \simeq 1 + 0.325 \frac{1}{R}.$$  

Notice that in order to obtain the result, we made use of the relation $S_M / V_M = 2/R$. We now rewrite Eq. (50) as

$$\Delta_R = 2\omega_D \exp \left(-\frac{1}{v_{sc}(R)}\right) = \Delta_B \exp \left(-\frac{1}{|v_0 g_B^B(1 + \frac{\pi}{4k^B_F R}) a(R)}\right) \exp \left(\frac{1}{|v_0 g_B^B|}\right).$$

In Fig. 5, we show the quantal and semiclassical gaps as a function of $R$ up to 6 nm for Al wires. We see that the semiclassical formula reproduces nicely the average behavior of the quantal pairing gap.

Equation (53) is fully semiclassical and therefore free from oscillations due to shell effects; for the approximate quantal gap normalized to the bulk, one could try to use, as in the case of films, an expression analogous to (41). However, due to the already mentioned strongly asymmetrically fluctuating DOS of the wire with respect to its mean value, this formula is, contrary to the film case, inaccurate and yields even qualitatively unacceptable results. The case of the wire clearly demonstrates well that taking in the gap equation average quantities like the semiclassical DOS does not necessarily mean that the result also averages the quantal gap.

### 3.3 Grains

Recent experiments [14] have triggered a lot of attention of the behavior of pairing gaps in metallic grains. Contrary to films and wires, grains do not have an infinite extension although the box potential can be a valid model. However, there exists a quite strong particularity in the fact that all s.p. energies are discrete and that the range of the force is limited by the Debye window $\mu \pm \hbar \omega_D$.

The gap equation assuming spherical symmetry reads, see Ref. [13] for more details,
\[ \Delta_{nl} = -(2l + 1) \sum_{n' l'} \nu_{n' l'} \nu_{n l}^* \frac{\Delta_{n' l'}}{2 \sqrt{(\varepsilon_{n' l'} - \mu)^2 + \Delta_{n' l'}^2}}, \]  
(54)

where \( n \) is the principal quantum number and \( l \) is the angular momentum. We consider only singlet pairing and no spin-orbit coupling at mean field level. \( \varepsilon_{nl} \) are the single particle energies of the system, i.e. the eigenvalue of an infinite spherical box when there is no pairing.

The corresponding s.p. wave functions are the spherical Bessel functions \( j_{nl}(r k_F(r)) \), where \( k_F(r) = \sqrt{2m \varepsilon_{nl}/r^2} \). Using these wave functions in Eq. (6) allows us to write the pairing matrix element as

\[ v_{n' l'} n l = -g_{nl} \int dr j_{n l}^2(k_F(r)r) j_{n l}^2(k_F(r)r) = -g \int dr \rho_{nl}(r) \rho_{n l}(r)r, \]  
(55)

where \( g_{nl} = \int dr j_{n l}^2(k_F(r)r) \).

The Debye window is so small that for grains of few nanometers radius only very few discrete s.p. levels enter into the window. The situation is well described by Croitoru et al. in Ref. [13]. So for box radii \( R < 10 \text{ nm} \) practically only diagonal matrix elements appear in Eq. (54).

In Fig. 6, we show the averaged gap \( \Delta = \sum_{nl} \Delta_{nl} u_{nl} v_{nl}/ \sum_{nl} u_{nl} v_{nl} \) for Sn grains as a function of the grain radius \( R \) in the range between 3.0 nm and 3.2 nm (\( u_{nl} v_{nl} = \Delta_{nl}/2 \sqrt{(\varepsilon_{nl} - \mu)^2 + \Delta_{nl}^2} \) is the pairing tensor strongly peaked around the chemical potential). The numerical parameters to do the calculations have been taken from Ref. [13]. We clearly see, as a function of \( R \), how one level after the other enters and leaves the Debye window. This is indicated by the well delimited and almost horizontal plateaus. In the limit of purely diagonal matrix element, given the small Debye window around the Fermi energy, we have that \( \varepsilon_{nl} \approx \mu \), so we can write

\[ \Delta_{nl} = -(2l + 1) \sum_{n' l'} \nu_{n' l'} \nu_{n l}^* \frac{\Delta_{n' l'}}{2 \sqrt{(\varepsilon_{n' l'} - \mu)^2 + \Delta_{n' l'}^2}}, \]  
(56)

Using a local contact interaction, we obtain the expression of the matrix element given in Eq. (6). The corresponding semiclassic version of the matrix element reads

\[ v_l(E, E) = -g \int d^3 \rho_{El}(r), \]  
(57)

where \( \rho_{E l}(r) \) is the expression for the density of individual levels (the ‘on the energy shell density’) as derived in Refs. [28,29]

For \( d = 0.003 \text{ nm} \), we obtain very good agreement with the quantal values for various values of \( l \) with this single parameter \( d \), as it can be seen in Fig. 7. The agreement deteriorates slightly for higher \( l \)-values, but at the same time the values of the matrix elements decrease so that the slight inaccuracy is not very important. Experimentally, one cannot measure the gap for each \( l \)-value separately, only some average at the Fermi energy is accessible. For the quantal gaps, we do that in taking an average with the already used pairing tensor \( \kappa = \mu \) which is peaked at the Fermi surface. Semiclassically we replace \( l \) by its mean value \( \langle l \rangle = \frac{1}{2} k_F R \) so we get

Fig. 6 Strong zoom for gap of Sn of spherical grain rescaled to the bulk value of the pairing gap \( \Delta_B \). The plateau’s correspond to single levels entering and leaving the Debye window. Notice that most of the points overlaps due to the very short step in the radius we used in order to produce the figure

\[ \rho_{E, l}(r) = \frac{l}{8\pi^2 r^2 g_{E,l}} \left( \frac{2m}{h^2} \right)^{1/2} \left[ E - V(r) - \frac{\hbar^2 l^2}{2mr^2} \right]^{-1/2} \times \Theta(E - V(r) - \frac{\hbar^2 l^2}{2mr^2}), \]  
(58)

\[ g_{E,l} \] is the corresponding level density obtained from above expression for the on the energy shell density by integration

\[ g_{E,l} = \int d^3 \rho_{E,l}(r), \]  
(59)

where \( k_F = \sqrt{2mE/\hbar^2} \) is the momentum at energy \( E \).

The integral in Eq. (57) diverges as often happens with semiclassic expressions which have to be considered as distributions and one has to regularise them.

In this case, we introduce a cut off value \( d \) and we get

\[ v_l(E, E) = -g \frac{1}{8\pi^2 k_F^2} \frac{k_E^3}{R^2 - l^2} \ln \left( \frac{(Rk_E - l)}{k_E d(Rk_E + l)} \right), \]  
(60)
Fig. 7 Semiclassic (solid line) and quantal matrix elements (symbols) as a function of \( R \) for different values of \( l \) with single parameter \( d \) in expression (60).

Fig. 8 Gap for the sphere as a function of radius \( R \) (circles) is shown together with the semiclassical result. The squares correspond to the hemisphere with the same radius \( R \). Why sphere and semi-sphere give very similar results is explained in the text. The broken yellow line indicates the asymptotic value

\[
\nu(E, E) = \frac{g}{3\pi} \frac{1}{R^3} \ln \left( \frac{R}{6d} \right).
\] (61)

By replacing this expression in Eq. (56), we get a simple expression for the pairing gap. Since this formula is derived under the diagonal approximation in the limit of large \( R \) the semiclassical gap vanishes as the matrix element. To avoid that we add to Eq. (56) the gap of the bulk \( \Delta_B \).

In order to numerically validate the formula, we take the parameters for Sn [13]: \( gN(0) = 0.25 \); \( k_F = 16.4 \) nm\(^{-1} \); \( \hbar^2/(2m) = 38.1 \) meV nm\(^2 \), leading to a bulk value of the pairing gap of \( \Delta_B = 0.61 \) meV. In Fig. 8, we compare the results obtained using semiclassical approximation discussed above with the quantal results obtained repeating the calculations of Ref. [13].

The experimental setup to study nanograins is actually formed by hemisphere and not full spheres [14]. We have thus repeated the quantal calculation for such a geometry and reported the results in Fig. 8. Actually sphere (circles) and hemisphere (squares) give very similar results. This stems from the fact that in hemispheres the level density is half of the one of the sphere. However, also the volume is half, so that both effects cancel. A detailed study of the hemisphere is given in Appendix A. For the hemisphere exist some experimental values in Ref. [30] in the range 18 nm < \( R \) < 30 nm. Actually it is not explained in [30] from where the experimental values come from. In the original paper by Bose et al. [14] the values are always shown with respect to the average, however, the average is never displayed.

Let us conclude concerning the results of electronic nano-devices. Besides for films, the semiclassical Weyl description is faced with some difficulties stemming from the fact that for system-sizes of only a few nanometers the Debye window lets penetrate, as a function of varying sizes, discrete levels only one by one, rendering the system highly quantal. For small metallic grains this difficulty could be circumvented because what counts in such cases is finally the size dependence of the pairing matrix elements for which good semiclassical expressions exist. The case of metallic nano-wires is intermediate. Discrete transverse levels are embedded in the continuum of the infinite wire. This makes a semiclassical approach particularly demanding because the quantal fluctuations around the average go mostly to one side and not symmetrically to both sides as in the case of films. We could find a very accurate global correction factor to the semiclassical expression with which the quantal results are perfectly averaged. This then also yields very good reproduction of the existing experimental data. In the case of films the quantal fluctuations are symmetric around the average and small enough, so that the semiclassical Weyl approach yields a perfect average of the fluctuating gaps. Then the increase of the gaps with decreasing sizes is clearly due to the increase of the influence of the surface pressure giving rise to an increase of the DOS.

4 Conclusions

The BCS approximation is a quite valid approximation for steep mean field potentials where the surface width is small compared to the total extension of the system as this is the case in most realistic systems as, e.g., electronic nano-devices and nuclei. Further, we have demonstrated that semiclassical methods, as the Weyl approximation for box potentials and the Thomas–Fermi approximation for finite potentials with a distributed surface, are very useful tools to reveal generic average surface and size dependences of systems so largely different as are nano-sized electronic devices. Of course, in those ultrasmall systems strong shell effects are
generally present, but eventually they can be added perturbatively and are, in any case, not responsible for the underlying, sometimes quite subtle, surface and size dependences. For instance one of the main agents of the increase of pairing with decreasing sizes is the fact that the increasing influence of the surface pressure with decreasing size compresses the systems and, thus, the Fermi momentum, i.e. the level density, increases and, consequently, the gap. This is very clearly born out in very thin electronic films where quantal shell effects are not very pronounced. As soon as the dimensions are further reduced as in electronic wires and grains where discrete levels are involved, the quantal fluctuations raise very strongly.

In such cases a new aspect has to be considered, namely that the Debye window is usually so small that for very small diameters of the systems, it may happen that only one or at most very few discrete levels enter the Debye-widow at once. This naturally becomes then a highly quantal situation where semiclassical methods are not very well adopted. Fortunately in these cases the gap field becomes practically diagonal and semiclassically the pairing matrix elements can again be very well reproduced with Thomas–Fermi like approaches, see Eq. (29). Indeed, we could show that the average size dependence of the pairing matrix elements in these cases the gap field becomes practically diagonal and semiclassically methods are not very well adopted. Fortunately in these cases the gap field becomes practically diagonal and the main agent of the size dependence of pairing is given solely by the size dependence of the pairing matrix elements [13]. In earlier works, we have shown that the average size behaviour of the pairing matrix elements can again be very well reproduced with Thomas–Fermi like approaches, see Eq. (29). Indeed, we could show that the average size dependences of gaps of spherical grains as well as of grains of hemispherical shapes can very well be reproduced with our semi-classical methods.

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Appendix A: Quantal study of a free particle in a hemisphere

The Schrödinger equation for a free particle confined in a half-sphere of radius $R$ read

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_{nlm}(r, \theta, \phi) = E \psi_{nlm}(r, \theta, \phi). \quad (A1)$$

The problem has very specific boundary conditions i.e. $\psi_{nlm}(r, \theta, \phi)$ is equal to zero at the edges of the half sphere. Before entering in a more detailed discussion, it is interesting to specify the system of reference. $r$ represent the radial distance from the centre of the sphere and it can take all values in the range $r \in [0, R]$, $\theta$ is the angle formed by $r$ with the axis of symmetry of the half sphere it goes from $\theta \in [0, \pi/2]$. The value $\theta = 0$ indicates a point on the top of the half-sphere, the value $\theta = \pi/2$ is placed on the disk closing the bottom of the half-sphere. $\phi$ is the angle formed by the projection of $r$ on $xy$-plane and it spans from 0 to $2\pi$.

The boundary conditions can be then translated as

$$\left\{ \begin{array}{l} \psi_{nlm}(R, \theta, \phi) = 0 \quad \theta \neq \frac{\pi}{2}, \\ \psi_{nlm}(r, \frac{\pi}{2}, \phi) = 0 \quad \theta = \frac{\pi}{2}, \end{array} \right.$$

these two conditions take into account the fact that the wavefunction is zero on the hemisphere and the disk delimiting the Hilbert space. To solve such a problem, we use the usual ansatz of $\psi_{nlm}(r, \theta, \phi) \propto u_{nl}(r) Y_{lm}(\theta, \phi)$, \quad (A2)

where $nlm$ are the quantum number of the system. $Y_{lm}(\theta, \phi)$ is the spherical harmonic. Notice we neglect spin terms since there is no spin-orbit coupling and the terms simply factorise.

We replace Eq. (A2) in Eq. (A1) and we get

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right] u_{nl}(r) = E_{nl} u_{nl}(r). \quad (A3)$$

By defining $k_{nl}^2 = \frac{2m}{\hbar^2} E_{nl}$ and performing simple manipulations, we obtain the Bessel equation whose solution are the spherical Bessel functions $u_{nl}(r) = j_l (k_{nl} r)$.

By imposing the first set of boundary conditions, i.e. $u_{nl}(R) = 0$, we obtain the discretisation of the eigen-spectrum. This condition is angle independent. In the case of a closed half-sphere, we also need to impose that the wave function is zero on the bottom disk closing the space. This condition should be valid for any value of $r$ and fixed $\theta = \pi/2$.

As such we have to impose this on the angular part of the wave function

$$Y_{lm}\left(\frac{\pi}{2}, \phi\right) = 0. \quad (A4)$$

This is achieved simply by selecting the associated Legendre polynomial that are odd $P_l^m(\cos \theta)$, or in other words they have a node on the $\theta = \pi/2$ plane. This conditions is respected for all polynomials so that $l + m$ is an odd number ($l = 0$ excluded). As a consequence, we can solve the half-sphere problem using the same methodology used to solve the sphere, apart from the extra selection rule on the quantum number used to build the basis.
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