Energetics of an interacting electron system on a surface

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ABSTRACT

We present some properties of an interacting N-fermion system on a cylindrical surface focusing in the quantum mechanical size effects of the ground-state observables. We use an effective zero-range two-fermion interaction which allows for an analytical Hartree–Fock approach. Within this model, quantum size effects can be understood as a consequence of filling states in the Fermi sea in which naturally arises a clear dependence on the Fermi momentum and the cylinder radius. Particularly, the model shows that the difference between the surface and bulk energies does not depend on the strength interaction. A relationship between the chemical potential and the bulk energy is analytically derived. The approach is also suitable for carbon nanotubes.

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1. Introduction

Quantum mechanics in one-dimensional N-particle systems has been historically studied because its simplicity for some two-body interactions, which allow for analytical solutions of the many-body problem. Particularly, it is the case of the N-boson(fermion) systems with two-body contact interactions [1,2]. Such solutions are useful in quantum statistical physics [3]. The contact interaction has also been used within the density functional theory [4] aiming to provide more insights to a better understanding of this theory [5]. It may be of importance in more involved quantum-mechanical N-body problems with higher dimensions. Quantum mechanics in two-dimensions (2D) differs in many aspects from the one-dimensional (1D) and three-dimensional (3D) cases. Particularly, the centrifugal barrier is zero or positive in 3D, whereas in 2D the s-wave barrier is in fact negative. Consequently, two particles in 2D are at the threshold of binding even when they do not interact, i.e., an infinitesimal amount of attraction produces a bound state. In 3D occurs a complete different situation, since it is well-known that a finite amount of attraction is required to produce two-body bound states. The effect of the dimension in the quantum many-body problem is still an interesting issue. Particularly, a large theoretical avenue has been opened for low dimensional quantum-mechanical systems since the phenomenal nanoscience growth [6]. For example, recently the jellium model in condensed matter [7] has been applied to calculate the energy in a finite two-dimensional fully spin-polarized electron gas in an analytical way [8], aiming the investigation of how the energy converges towards the thermodynamic bulk limit.

From the Hugenholtz–Van Hove theorem [9], valid for an interacting N-body system and for zero temperature, the chemical potential reads

$$\mu = \frac{E + P\Omega}{N},\qquad(1)$$

where E, P and Ω are the total energy, pressure and volume (in the 3D case) or area (in the 2D case) of the system, respectively. By studying general average properties of a three-dimensional liquid system, the authors of [10] found a way to describe the chemical potential in terms of a bulk energy and a potential step at the surface. It has been done by extending the Budd–Vannimenus theorem [11] to include volume effects. The study of [10] allows the separation of volume and surface effects in consistency with Eq. (1). In short, Eq. (1) can be rewritten as

$$N\mu = E_b + P\Omega \equiv E_b + E_s,\qquad(2)$$

where one can identify $P\Omega$ as a surface energy E_s. In accordance with [10] the surface potential step also accounts for the pressure. Furthermore, the authors of [10] show that the difference between μ and the energy per particle is exactly the electrostatic potential step at the surface. The authors used this finding to investigate a one-dimensional integrable model for the BCS-BEC crossover in an analytical way. Surface energy effects have been also studied for finite metallic nanowires [12] and for transition metal carbides [13].

It is also interesting to have at hand a 2D model for interacting N-fermion systems, that allow an analytical treatment of the many-body properties. In particular, it is desirable to have a model that the bulk and surface effects could be seen separately not only for a flat layer, but also for a cylindrical surface. The variety of two-dimensional nanostructures is a rich source for materials to tailor electronic nanodevices properties. For example: carbon nanotubes, which ideally provide a

nano-cylinder where electrons in the p-wave orbitals have a high mobility and are the basis for the description of the optical and electronic properties of these materials [14]. Therefore, a model that catches the relevant theoretical aspects of the interacting quantum mechanical N-fermion system not constrained by a specific engineering application, can be useful and the basis for broad practical usages.

The understanding of the energetics of the fermion gas constituted by high mobility electrons on the surface, either flat or cylindric, is essential to design the properties of layered materials. In this respect, an analytical model can play an essential role. In particular, it is worthwhile to separate the contributions from kinetic and potential energies of the high mobility electrons to the bulk and surface parts of the total gas energy. It is reasonable to expect that the potential energy contribution to the bulk and surface energies is equal in 2D, because the high mobility fermions are constrained to one layer where the effective forces among them act. In this case the equality between the potential energy contributions to the bulk and surface energies is evident for effective interactions with a range much smaller than the cylinder radius. This equality should be quite universal for short-range forces as short range correlations are essentially unaltered when the layer is folded to form the cylinder. However, this general physical trend is not valid for the kinetic energy contributions to the surface and bulk energies when the flat surface is folded to form a cylindric one.

The total kinetic energy of the high mobility fermions is strongly dependent on the nanotube radius. Constraining the fermions to the surface of a cylinder, one dimension becomes compact, and the quantum system reacts with states quantized according to the requested periodic boundary condition. This is not essential at short distances but changes the infrared or long distance behaviour of the one-body density, while the two-body density at distances smaller than the radius are not sensitive to the folding of the 2D layer. All these features are indeed verified analytically in the schematic model we will discuss in the following.

In this work we discuss the bulk and surface energy contributions for a 2D electron interacting system on a cylindrical surface. We will explore a recent model based on nonrelativistic quantum field theory [15]. To obtain the properties of the ground state, the Hartree–Fock approximation is performed analytically for an effective zero-range two-body interaction given in cylindrical coordinates (z, θ) by

$$V(z, \theta) = -\frac{\lambda}{R}\delta(z)\delta(\theta), \tag{3}$$

where R is the radius of the cylinder and λ is an unknown strength. In the model, one assumes for fermions of mass m a simple Fermi surface defined by a momentum k_F. This model [15] was applied to investigate carbon nanotube (CNT) properties and λ was eliminated in favour of the experimental graphene work function value of 4.8 eV [16]. The graphene limit is achieved when one takes the limit of R going to infinity.

This work is organised in four sections. In Section 2, we present the field-theoretical model for the interacting fermion gas on the 2D cylindrical surface and the thermodynamical quantities analytically derived. In Section 3, we analyse our model by presenting quantitative results for the energetics of the fermionic system. In Section 4, we conclude with a summary of the main results.

2. Model

Here we follow the model [15] to compute the thermodynamical quantities. Our starting point is the fermion Hamiltonian operator with two-body interactions

$$H = \sum_{spin} \int d\vec{r} \left[\frac{1}{2m}\nabla\psi_s^\dagger\left(\vec{r}\right) \cdot \nabla\psi_s\left(\vec{r}\right) + \frac{1}{2}\int d\vec{r}'\psi_{s_1'}^\dagger\left(\vec{r}\right)\psi_{s_2'}^\dagger \right. \tag{4}$$
$$\left. \times \left(\vec{r}'\right)\left\langle s_1's_2'|v\left(\vec{r}'-\vec{r}\right)\right|s_1s_2\right\rangle \psi_{s_2}\left(\vec{r}'\right)\psi_{s_1}\left(\vec{r}\right) \right],$$

where the local two-body potential can depend also on the spin state, with matrix elements $\left\langle s_1's_2'|v\left(\vec{r}'-\vec{r}\right)\right|s_1s_2\right\rangle$. The fermionic field operators are quantized according to the standard anticommutation rules, i.e.,

$$\left\{\psi_{s'}\left(\vec{r}'\right), \psi_s^\dagger\left(\vec{r}\right)\right\} = \delta_{s's}\delta\left(\vec{r}'-\vec{r}\right) \quad \text{and} \quad \left\{\psi_{s'}\left(\vec{r}'\right), \psi_s\left(\vec{r}\right)\right\} = 0 , \tag{5}$$

where the subindex s indicates the spin state. In the model [15] the effective potential acting on the singlet spin states has matrix elements given by:

$$\left\langle s_1's_2'|v\left(\vec{r}'-\vec{r}\right)\right|s_1s_2\right\rangle = \frac{\lambda}{2}\left\langle s_1's_2'|00\right\rangle\delta\left(\vec{r}'-\vec{r}\right)\left\langle 00|s_1s_2\right\rangle, \tag{6}$$

where $\langle s_1s_2|SM\rangle$ is the Clebsch–Gordan coefficient. The Hartree–Fock (HF) treatment of the ground state was detailed in ref. [15] and here we just highlight the main thermodynamical quantities at zero temperature for $N \to \infty$. The higher order correlations are not taken into account in the HF approximation, but effectively they are included in the equation of state by fitting the strength of the potential (λ) to the graphene work-function, which obviously demands the full correlated electron wave function to be calculated properly. The value of λ may be eliminated in favour of any chosen many-fermion physical quantity.

The thermodynamical quantities are presented in the following. The number of electrons on a nanotube surface is given by

$$N = \frac{2L}{\pi}\sum_{n=-n_{max}}^{n_{max}}\left(k_F^2 - \frac{n^2}{R^2}\right)^{1/2}, \tag{7}$$

where n_{max} is the highest integer smaller than $k_F R$, n/R is the angular wave number k_θ and L is the length of the cylinder. Hereafter we will use $|n|$ in the summations. The electron surface density is

$$\sigma = \frac{N}{A}, \tag{8}$$

with $A = 2\pi RL$ being the area of the cylinder surface. The kinetic energy of the particle in the Fermi level is

$$T_F = \frac{k_F^2}{2m} \tag{9}$$

where k_F is the Fermi momentum. The average total bulk energy is obtained from the matrix element of the Hamiltonian operator in the ground state, namely, $\langle H \rangle = \langle T \rangle + \langle V \rangle$. The bulk energy is the expectation value of Eq. (4), which in the HF approximation is given by:

$$E_b = \langle H \rangle = \frac{L}{3\pi m}\sum_{|n| \leq n_{max}}\left(k_F^2 + 2\frac{n^2}{R^2}\right)\sqrt{k_F^2 - \frac{n^2}{R^2}} + \frac{\lambda}{2}\sigma N \tag{10}$$

which is the total kinetic and potential energies of the electrons in the system. The surface energy, obtained from the pressure, is given by

$$E_s = -\frac{\partial\langle H \rangle}{\partial A}A = P.A = \frac{2}{3}\frac{L}{\pi m}\sum_{|n| \leq n_{max}}\left(k_F^2 - \frac{n^2}{R^2}\right)^{\frac{3}{2}} + \frac{\lambda}{2}\sigma N \tag{11}$$

where P is the pressure. It is convenient here to introduce a dimensionless parameter x as

$$x = k_F R, \tag{12}$$