Trapping effect of periodic structures on the thermodynamic properties of Fermi and Bose gases

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We report the thermodynamic properties of Bose and Fermi ideal gases immersed in periodic structures such as penetrable multilayers or multitubes simulated by one (planes) or two perpendicular (tubes) external Dirac comb potentials, while the particles are allowed to move freely in the remaining directions. Although the bosonic chemical potential is a constant for $T < T_c$, a non decreasing with temperature anomalous behavior of the fermionic chemical potential is confirmed and monitored as the tube bundle goes from 2D to 1D when the wall impenetrability overcomes a critical value. In the specific heat curves dimensional crossovers are very noticeable at high temperatures for both gases, where the system behavior goes from 3D to 2D and latter to 1D as the wall impenetrability is increased.

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I. INTRODUCTION

Non-relativistic quantum fluids (fermions or bosons) constrained by periodic structures, such as layered or tubular, are found in many real or man-made physical systems. For example, we find electrons in layered structures such as cuprate high temperature superconductors or semiconductor superlattices, or in tubular structures like organo-metallic superconductors.

On the experimental side, there are a lot of experiments around bosonic gases in low dimensions, such as: BEC in 2D hydrogen atoms, 2D bosonic clouds of rubidium, superfluidity in 2D $^4$He films, while for in 1D we have the confinement of sodium, to mention a few.

Meanwhile, for non-interacting fermions there are only a few experiments, for example, interferometry probes which have led to observe Bloch oscillations.

To describe the behavior of fermion and boson gases inside this symmetries, several works have been published. For a review of a boson gas in optical lattices see, and for fermions is very complete. Most of this theoretical works use parabolic, sinusoidal and biparabolic potentials, with good results only in the low particle energy limit, where the tight-binding approximation is valid.

Although in most of the articles mentioned above the interactions between particles and the periodic constrictions are taken simultaneously in the system description, the complexity of the many-body problem leads to only an approximate solution. So that the effects of interactions and constrictions in the properties of the system, are mixed and indistinguishable.

In this work we are interested in analyzing the effect of the structure on the properties of the quantum gases regardless of the effect of the interactions between the elements of the gas, which we do as precisely as the accuracy of the machines allows us to do.

This paper unfolds as follows: in Sec. 2 we describe our model which consists of quantum particles gas in an infinitely large box where we introduce layers of null width separated by intervals of periodicity $a$. In Sec. 3 we obtain the grand potential for a boson and for a fermion gas either inside a multilayer or a multitube structure. From these grand potentials we calculate the chemical potential and specific heat, which are compared with the properties of the infinite ideal gas. In Sec. 4 we discuss results, and give our conclusions.

II. QUANTUM GASES WITHIN MULTILAYERS AND MULTITUBES

We consider a system of $N$ non-interacting particles, either fermions or bosons, with mass $m_b$ for bosons or $m_f$ for fermions respectively, within layers or tubes of separation $a_i$, $i = x$ or $y$, and width $b$, which we model as periodic arrays of delta potentials either in the $z$-direction and free in the other two directions for planes, and two perpendicular delta potentials in the $x$ and $y$ directions and free in the $z$ one for tubes. The procedure used here is described in detail in Refs. and for a boson gas, where we model walls in all the constrained directions using “Dirac comb” potentials. In every case, the Schrödinger equation for the particles is separable in $x$, $y$ and $z$ so that the single-particle energy as a function of the momentum $k = (k_x, k_y, k_z)$ is $\varepsilon_k = \varepsilon_{k_x} + \varepsilon_{k_y} + \varepsilon_{k_z}$. For the directions where the particles move freely we have the customary dispersion relation $\varepsilon_{k_i} = \hbar^2 k_i^2/2m_i$, with $k_i = 2\pi n_i/L$, $n_i = \pm 1, \pm 2, \ldots$, and we
are assuming periodic boundary conditions in a box of size L. Meanwhile, in the constrained directions, z for planes and x, y for tubes, the energies are implicitly obtained through the transcendental equation\(^{16}\)

\[
(P_i/\alpha_i a_i) \sin(\alpha_i a_i) + \cos(\alpha_i a_i) = \cos(k_i a_i),
\]

(1)

with \(\alpha_i^2 = 2 m_i \varepsilon_i / \hbar^2\), and the dimensionless parameter \(P_i = m_i V_0 a_i / \hbar^2\) represents the layer impenetrability in terms of the strength of the delta potential \(V_0\). We redefine \(P_i = (m_i V_0 \lambda F_0 / \hbar^2)(\alpha_i / \lambda F_0) \equiv P_{0i}(\alpha_i / \lambda F_0)\), where \(\lambda F_0 \equiv \hbar / \sqrt{2\pi m_i k_B T F_0}\) is the thermal wavelength of an ideal gas inside an infinite box, with \(k_B T F_0 = E F_0 = (3\pi^2)^{2/3}(\hbar^2/2 m_i) \rho^{2/3}\) the Fermi energy and \(\rho = (k_B T F_0)^{3/2}/3\pi^2 a^2 (\hbar^2/2 m a^2)^{3/2}\) is the density of the gas.

The energy solution of Eq. (1) for boson gases has been extensively analyzed in Refs.\(^{13,14}\) and\(^{15}\), where the allowed and forbidden energy-band structure is shown, and the importance of taking the full band spectrum has been demonstrated.

### III. THERMODYNAMIC PROPERTIES OF QUANTUM GASES IN MULTILAYERS AND IN MULTITUBES

Every thermodynamic property may be obtained starting from the grand potential of the system under study, whose generalized form is\(^{17}\)

\[
\Omega(T, L^3, \mu) = U - TS - \mu N = \delta_{n,-1} \Omega_0 - \frac{k_B T}{a} \sum_{k=0} \ln \{ 1 + a \exp[-\beta(\varepsilon_k - \mu)] \},
\]

(2)

where \(a = -1\) for bosons, 1 for fermions and 0 for the classical gas, \(\delta\) is the Kronecker delta function and \(\beta = 1/k_B T\). The ground state contribution \(\Omega_0\), which is representative of the Bose gas, is not present when we analyze the Fermi gas.

For a boson gas inside multilayers we go through the algebra described in\(^{13,14}\), and taking the thermodynamic limit one arrives to

\[
\Omega(T, L^3, \mu) = k_B T \ln(1 - \exp[-\beta(\varepsilon_0 - \mu)])
\]

\[
- \frac{1}{\beta^2} \frac{L^3 m}{2(2\pi)^2 \hbar^2} \int_{-\infty}^{\infty} dk_z g_2 \{ \exp[-\beta(\varepsilon_k - \mu)] \}.
\]

(3)

Meanwhile, for a fermion gas we get

\[
\Omega(T, L^3, \mu) = -2 \frac{L^3 m}{(2\pi)^2 \hbar^2} \int_{-\infty}^{\infty} dk_z \ f_2 \{ \exp[-\beta(\varepsilon_k - \mu)] \},
\]

(4)

where \(g_2(t)\) and \(f_2(t)\) are the Bose and Fermi-Dirac functions\(^{17}\). The spin degeneracy has been taken into account for the development of Eq. (3).

On the other hand, for a multilayer structure we have

\[
\Omega(T, L^3, \mu) = k_B T \ln[1 - e^{-\beta(\varepsilon_0 - \mu)}]
\]

\[
- \frac{L^3 m^{1/2}}{(2\pi)^{3/2} \hbar^{3/2}} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y g_{3/2} (e^{-\beta(\varepsilon_k + \varepsilon_{k_y} - \mu)})
\]

(5)

for a boson gas, and

\[
\Omega(T, L^3, \mu) = -2 \frac{L^3 m^{1/2}}{(2\pi)^{3/2} \hbar^{3/2}} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y f_{3/2} \{ \exp[-\beta(\varepsilon_k + \varepsilon_{k_y} - \mu)] \}
\]

(6)

for a fermion gas.

For calculation matters, it is useful to split the infinite integrals into an number \(J\) of integrals running over the energy bands, taking \(J\) as large as necessary to acquire convergence.

#### A. Chemical potential and specific heat

For a gas inside a multilayer structure, the particle number \(N\) is directly obtained from Eqs. (3) and (4). Important characteristics can be extracted, such as the critical temperature for a condensating boson gas and the influence of
the system parameters on it, \( a \) and \( P_0 \), already reported in Refs.\(^{13,14}\). But for the case of a fermion gas, we focus on the chemical potential since it is closely related to the Fermi energy of the system. In this case the number equation is

\[
N = 2 \frac{L^3}{(2\pi)^{5/2}} \frac{m L^1/2}{\hbar^{1/2}} \int_{-\infty}^{\infty} dk_z \ln\left\{ 1 + \exp\left[ -\beta (\varepsilon_{k_z} - \mu) \right] \right\},
\]

from which we are able to numerically extract the Fermi energy of the system, which corresponds to the chemical potential for \( T = 0 \), over the Fermi energy of the IFG \( E_{F0} = (\hbar^2/2m)k_F^2 = (\hbar^2/2m)4\pi^2/\lambda_{F0} \), namely \( E_F/E_{F0} \), as a function of the impenetrability parameter \( P_0 \), whose behavior corresponds to a monotonically increasing curve as \( P_0 \) increases, being more evident for smaller values of \( a/\lambda_{F0} \). Another important feature is the chemical potential of the system over its Fermi energy, \( \mu/E_F \), which is probably the feature that attracts greater attention due to its anomalous behavior shown in Fig. 2, which shows up as an unexpected small hump.

Another interesting characteristic is that the chemical potential over the IFG Fermi energy in every case is lifted as \( P_0 \) increases due to the presence of the layers, in the same way as the chemical potential of the boson gas started above zero.

The specific heat of a boson gas has been reported in Ref.\(^{13–15}\) where we can observe a transition from a 3D system to a 2D one, which becomes evident for certain parameter values and sufficiently high temperatures. At this point is where the advantages of summing over a great amount of allowed energy bands shows its relevance.

Meanwhile, the specific heat for a fermion gas inside layered arrays is obtained going through the derivatives of

\[
\text{FIG. 1: (Color online) Chemical potential as a function of } T/T_{F0} \text{ for planes with } P_0 = 100 \text{ and different values of } a/\lambda_{F0}.
\]

We make a similar procedure for the boson an fermi gases inside a multtube structure, the first one being reported in\(^{15}\). But for a fermion gas we start from the equation

\[
N = 2 \frac{L^3}{(2\pi)^{3/2}} \frac{m^{1/2}}{\hbar^{1/2}} \frac{1}{\beta^{1/2}} \int_{-\infty}^{\infty} dk_z f_{1/2} \{ \exp[ -\beta (\varepsilon_{k_z} + \varepsilon_{k_y} - \mu)] \}
\]

and extract the chemical potential over the Fermi energy of the system, \( \mu/E_F \), which is probably the feature that attracts greater attention due to its anomalous behavior shown in Fig. 2 which shows up as an unexpected small hump.

Another interesting characteristic is that the chemical potential over the IFG Fermi energy in every case is lifted as \( P_0 \) increases due to the presence of the layers, in the same way as the chemical potential of the boson gas started above zero.

The specific heat of a boson gas has been reported in Ref.\(^{13–15}\) where we can observe a transition from a 3D system to a 2D one, which becomes evident for certain parameter values and sufficiently high temperatures. At this point is where the advantages of summing over a great amount of allowed energy bands shows its relevance.

Meanwhile, the specific heat for a fermion gas inside layered arrays is obtained going through the derivatives of
Eqs. (3) and (6), leading, after some algebra, to

\[
\frac{C_V}{Nk_B} = \frac{L^3}{N\left(2\pi\right)^2} \frac{m}{\hbar^2} \left\{ \frac{4}{\beta} \int_{-\infty}^{\infty} dk_x f_2 \left\{ \exp\left[-\beta(\varepsilon_{k_z} - \mu)\right] \right\} \right.
\]
\[
+ 2 \int_{-\infty}^{\infty} dk_x \ln\left\{ 1 + \exp\left[-\beta(\varepsilon_{k_z} - \mu)\right] \right\} \left\{ 2\varepsilon_{k_z} - \mu + T \frac{d\mu}{dT} \right\}
\]
\[
+ 2\beta \int_{-\infty}^{\infty} dk_x \frac{\varepsilon_{k_z}}{\exp\left[\beta(\varepsilon_{k_z} - \mu)\right]} - 1 \right\} \quad (9)
\]

for multiplanes, and

\[
\frac{C_V}{Nk_B} = \frac{2L^3}{N\left(2\pi\right)^{5/2}} \frac{m^{1/2}}{\hbar} \left( \frac{\beta^{1/2}}{2} \right) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_x dk_y \left[ f_{1/2}(e^{-\beta(\varepsilon_{k_x} + \varepsilon_{k_y} - \mu)})
\right.
\]
\[
+ (2\varepsilon_{k_x} + 2\varepsilon_{k_y} - \mu + T \frac{d\mu}{dT}) + \beta^{3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_x dk_y \varepsilon_{k_z} + \varepsilon_{k_y} \times
\]
\[
f_{-1/2}(e^{-\beta(\varepsilon_{k_x} + \varepsilon_{k_y} - \mu)}) \{ \varepsilon_{k_x} + \varepsilon_{k_y} - \mu + T \frac{d\mu}{dT} \}
\]
\[
+ \frac{3}{4\beta^{1/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_x dk_y f_{3/2}(e^{-\beta(\varepsilon_{k_x} + \varepsilon_{k_y} - \mu)}) \right\} \quad (10)
\]

for multitubes.

In Figs. 3 and 4 we show the behavior of the specific heat of layers with a separation among layers of \(a/\lambda_0 = 0.2\) and several impenetrability intensities \(P_0\), as a function of the temperature over the system’s Fermi temperature. It may be observed that, as the barriers disappear \((P_0 = 0)\), one recovers the IFG specific heat classical value, 3/2. It is also noticeable that as the value of \(a/\lambda_0\) diminishes, a dimensional crossover signature from 3D to 2D becomes evident, since the the first minimum (going from right to left) in the specific heat deepens towards a value \(C_V/Nk_B = 1.0\) and broadens as \(P_0\) increases. In Fig. 4 the dimensional crossover from 3D to 1D is very noticeable as the mentioned minimum drops down to the value 1/2 which corresponds to one-dimension.
FIG. 3: (Color online) Specific heat as a function of $T/T_{F0}$ for a fermion gas in multilayers.

FIG. 4: (Color online) Specific heat as a function of $T/T_{F0}$ for a fermion gas in multitubes.

IV. CONCLUSIONS

In summary, we have calculated the thermodynamic properties of ideal boson and fermion gases inside periodical structures. In our model the multilayers and multitubes are generated with Dirac-comb potentials in either one or two directions, while the particles are free in the remaining directions. Just by introducing the planes, the translational symmetry of the particles is broken. This fact reflects in every thermodynamic property of the constrained system. In particular, fermions in multi-tubes progress from a 3D behavior to that 2D and finally to 1D as the wall impenetrability is increased, which is observed in the curves of the specific heat as a function of temperature. There is a critical value of the wall impenetrability for which the system begins to behave in dimensions less than two, which
is signaled by the appearance of an anomalous chemical potential. Bosons in multitudes show similar dimensional crossover like that expressed by fermions, in addition to the Bose-Einstein condensation at temperatures below the critical temperature of an ideal Bose-gas with the same particle density.

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