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Perturbation theory for very long-range potentials

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ABSTRACT

Systems with very long-range interactions (that decay at large distances like $U(r)\sim r^{-l}$ with $l\leq d$ where d is the space dimensionality) are difficult to study by conventional statistical mechanics. Examples of these systems are gravitational and charged (non-electroneutral). In this work we propose two alternative methodologies to avoid these difficulties and capture some of the properties of the original potential. The first one consists of expressing the original potential in terms of a finite sum of hard-core Yukawa potentials. In the second one, the potential is rewritten as a damped potential, using a damping function with a parameter that controls the range of the interaction. These new potentials with finite ranges, which mimic the original one, can now be treated by conventional statistical mechanics methods.

1. Introduction

Description of systems interacting via the so-called long-range interactions (LRI) is an important statistical mechanics problem. These systems are found from very small to very large scales, for instance, in astrophysics [1–3], plasma physics [4,5], hidrodynamics [6], atomic physics [7] and, nuclear physics [8].

In order to use a precise definition of LRI between a pair of particles, that are a distance r apart, we consider the following: when the interaction potential between particles decays at long distances like $1/r^l$ in a space of d dimensions, the interaction can be considered to be long-range if $l\leq d$.

This definition is a consequence of considering the energy e of a given particle located at the center of a sphere of radius R with a homogeneous particle distribution in d-dimensions. In order to exclude the divergence that appears at very short distances, the energy of the neighboring particles located inside a sphere of radius δ is neglected, e is given by,

$$\begin{aligned} e &= \int_\delta^R \frac{\rho B}{r^l} d^d r = \rho B \Omega_d \int_\delta^R r^{(d-1)-l} dr \\ &= \frac{\rho B \Omega_d}{d-a}\left[R^{d-l} - \delta^{d-l}\right]; \qquad \text{if } l \neq d; \end{aligned} \tag{1}$$

where ρ is the generic particle density, B is a coupling constant which guarantees the correct energy dimensions, and Ω_d is the angular volume in the d-dimensional space. When R is increased, e remains finite only when $l>d$; such cases are the usual short-range interactions. The opposite corresponds to $l\leq d$, where energy diverges for an increasing volume; these are long-range interactions. Examples of different long-range potentials are shown in Fig. 1. Notice that this particular definition could be different in the context of fluids theory.

In statistical mechanics, most of the effort to obtain the equilibrium and non-equilibrium thermodynamic properties, has been concentrated on systems with short-range interactions. One of the main features of LRI systems is that their total energy, under the pairwise additive approximation, is non-extensive, and as a consequence, is also non-additive [9–14]. Therefore, the connection between Boltzmann–Gibbs (BG) statistical mechanics and classical thermodynamics is not straightforward, since the latter assumes that energy is an additive quantity [15]. To our knowledge, there is not a thermodynamic formalism (independent of a statistical mechanics approach) that allows this connection; however, it is possible to start from a non-extensive statistical mechanics and to obtain a non-extensive thermodynamic formalism.

Perhaps a non-extensive version of statistical mechanics could be a more natural theoretical frame to study LRI. A few proposals for BG statistical mechanics generalizations have been given [9,16,17], however none of them are unanimously accepted. Besides, the application of these generalizations to long-range potentials has been scarce. Another approach is to make adjustments to the BG formalism to study these systems [2,10,18].

In order to avoid the difficulties to treat LRI mentioned above, in this work we present a first naive approach, but general, in the sense that it can be applied to a great variety of long-range potentials in the frame of BG statistical mechanics. This methodology consists of rewriting a long-range potential as a short-range one, the latter being similar to the long-range potential in its graphical representation. We expect that this short-range potential recovers some features of the original one, however we realize that this path leads to a classical thermodynamics frame and we do not know if real systems with LRI are well represented by this thermodynamics.

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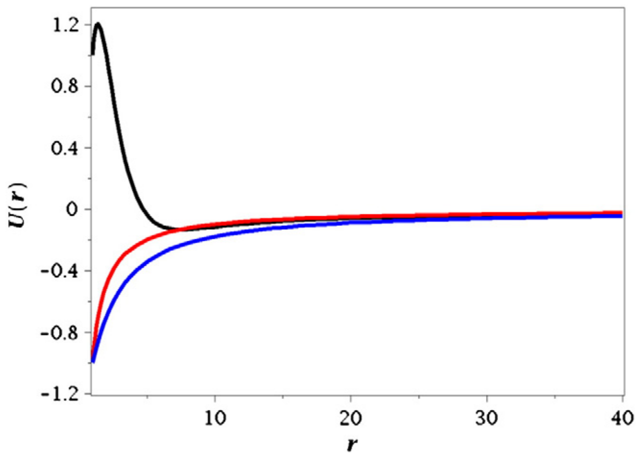

Fig. 1. Examples of different (repulsive and attractive) long-range potentials, that at long distances decay as $1/r$.

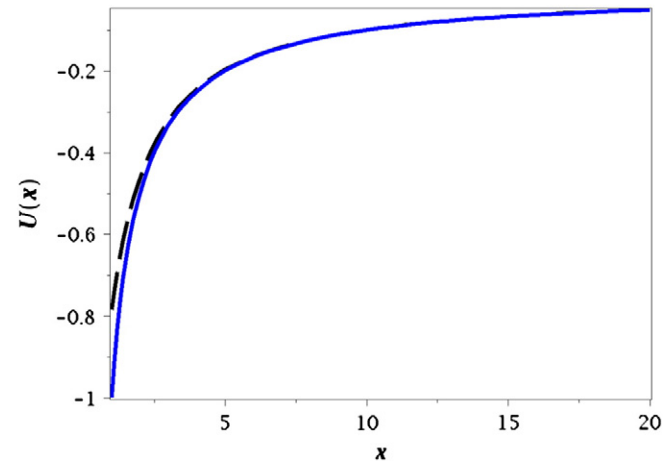

Fig. 2. The ETS potential with $\alpha^*=1$ (solid line) compared with $-1/x$ potential (dashed line). Long-range behavior is the same for both potentials.

More specifically our approach consists of expressing a given long-range potential as a) a finite sum of Yukawa potentials; b) a product of the potential with a damping function which depends on a parameter, that under a certain limit, the original potential is recovered.

We have selected the Discrete Perturbation Theory [19] (DPT) and the First-order Mean Spherical Approximation [20] (FMSA) to study these potentials. These theories have been successfully applied in the context of fluids and more recently in the soft matter field, and can be applied to a great variety of potentials.

As an illustrative example, we have chosen the gravitational potential due to the interaction between two identical spherical rotating bodies (ETS potential), obtained by Escamilla et al. [21]. More interesting models in the context of molecular liquids, could be, for instance, the Coulomb interactions.

This work is organized as follows. In Section 2, we give a brief description of the ETS potential and of the hard-core multi-Yukawa (HCMY) and damped potential approaches. In Section 3 we present internal energies, pressures, and vapor–liquid phase diagrams for the approximated potential. Finally, in Section 4 we give the main conclusions of this work.

2. Theory

2.1. The ETS potential

In the context of general relativity, within the weak-field limit methodology, an angular averaged potential due to the interaction between two identical spherical rotating bodies was proposed [21]. This interaction potential for hard-core spheres is given by $U^*(x) \equiv U(x)/|\epsilon_{min}|$, where:

$$U^*(x) = \begin{cases} \infty & \text{if } x < 1 \\ -\dfrac{1}{arctan(\alpha^*)} arctan(\alpha^*/x) & \text{if } x \geq 1; \end{cases} \tag{2}$$

with $\alpha^* \equiv J/Mc\sigma$, M is the mass, J is the angular momentum, c is the speed of light in vacuum, σ is the diameter of particles, $x = r/\sigma$ and ϵ_{min} is the potential evaluated at $x = 1$. This potential is purely attractive, nondivergent at short distances (for $x \to 0$, $1/\alpha^* arctan(\alpha^*/x) \to \pi/2$), and keeps its long-range nature satisfying the condition given by Eq. (1). Specific angular momentum α^* is a parameter which modulates the intensity of the interaction. The long-range behavior is the same for any finite value of α^*. For instance, in the limit of $\alpha^* \to 0$ the ETS potential goes to conventional $-1/x$ Newtonian gravitational interaction. In Fig. 2, the ETS and $-1/x$ potentials are shown; it can be noticed that the long-range behavior is the same for both of them.

To avoid the difficulties to evaluate thermodynamic properties for this long-range potential, we propose to rewrite the non-hard-core potential part as:

1) a finite sum of m Yukawa potentials,

$$\Phi_{MY}(x) = \sum_{i=1}^{m} = \epsilon_i^* \frac{exp[-\kappa_i^*(x-1)]}{x}; \quad multi-Yukawa\ approach, \tag{3}$$

with the energy and range parameters $\epsilon_i^* = \epsilon_i/|\epsilon_{min}|$ and κ_i^*, respectively, and

2) a damped potential, which consists of the product of the original potential and a damping function $f(\gamma,x)$,

$$\Phi_D(\gamma,x) = f(\gamma,x)\frac{U(x)}{|\epsilon_{min}|}; \qquad damped\ approach, \tag{4}$$

where γ is the damping parameter that can be selected in order to guarantee that the approximated potential mimics the original one.

2.2. First-order mean spherical approximation

The first-order mean spherical approximation was developed by Tang et al., [22] as an improvement of the mean spherical aproximation (MSA) [23].

The solution of the Ornstein–Zernike integral equation under MSA makes it possible to find analytical thermodynamic and structure expressions, which otherwise would require time-consuming numerical work. Despite these advantages, MSA may lose its solution in unstable regions [24]. An improvement of this theory is the first-order mean spherical approximation.

FMSA solves analytically the radial distribution function (RDF) to first order in terms of inverse temperature. Solutions obtained are explicit, simpler and always exist in unstable regions [24].

A successful application of FMSA theory was done by Tang et al., [22] to the Yukawa and HCMY potentials. A finite sum of Yukawa potentials can mimic other well-known potentials, like Lennard–Jones potential [20] or sticky hard spheres [25]; however, its efficacy for LRI like the ETS potential has never been tested to our knowledge. In this work we will approximate the ETS potential using HCMY potential to express it.