



## The relativistic virial theorem in plasma EOS calculations

A. Barshalom<sup>a</sup>, J. Oreg<sup>b,\*</sup>

<sup>a</sup>NRCN, Beer Sheva, P.O. Box 9001, Israel

<sup>b</sup>Artep Inc., Columbia, MD 21042, United states

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### ABSTRACT

A method is presented for accurate calculation of equation of state (EOS) for warm dense matter. The method extends an approach presented recently, based on the adjustment of the correlation energy to impose consistency between two pressure representations: the volume derivative of the free energy and the relativistic virial theorem. In this work we show that the free energy of any neutral system obeys a fundamental differential equation, which bypasses the correlation specifics and serves as a basis to enhance EOS approximations. Specifically, we start with LDA calculations and improve the results significantly using this equation with a boundary condition at the zero pressure point. The method retains the emphasis on thermal excitations, but connects to the appropriate results at low temperatures. It effectively compensates for simplifications, including the use of a spherical model to account for global solid structure effects. EOS and opacities are calculated on the same footing for low to high Z elements and in large domains of density and temperature without recourse to parametric fitting procedures. Excellent agreement is obtained with experiments. Finally the method is applied successfully to calculate EOS and opacities for mixtures. Results for C–H mixture are compared with other calculations.

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### 1. Introduction

Accurate equations of state (EOS) have become a crucial requirement for reliable simulations of laser-produced plasmas, inertial confinement fusion, astrophysics, planetary physics, and many other topics at the forefront of high energy density physics research [1]. Of particular interest are strongly coupled systems of partially ionized fluids at extremely high pressure and density [2], for which modeling becomes very difficult. In addition, for simulating the evolution of a system along experimental Hugoniot curves one requires accurate EOS in conditions ranging from normal density,  $\rho_0$ , to several times  $\rho_0$  and from room temperature to thousands of eV. To cope with these broad conditions, we need theories that emphasize thermal excitations [3,4], but which make contact with the proper results at low temperatures, like QEOS [5]. In addition, consistency requires that the same tools should be applicable for opacities and EOS, which are both essential components for simulations. For this purpose, we employ theories [4] that include detailed shape resonances (intermediate bound – continuum states) in a plasma environment, and use the well-known muffin tin spherical model [4]. This approach involves density functional simplifications where the local density

approximation (LDA) and its improvements, are used to incorporate exchange and correlation energies as explicit local density terms [6,7]. Whereas this theory reproduces the general properties of experimental data, the unavoidable use of approximations generate inaccuracies with some violating thermodynamic consistency and, therefore, require corrections to match observations. In practice, corrections to obtain agreement with experimental data rarely avoid empirical fits. A calibration, developed by More et al. [5] within a Thomas–Fermi (TF) model, works quite well in general, but uses a semi-empirical formula to improve the expression describing the bonding between atoms. Other methods that avoid empirical fits, e.g. Wang et al. [8], emphasize low temperature details but ignore the particulars of thermal excitations. To address this challenge we have recently presented the LCR approach [9] that is based on two pressure representations: one applies direct differentiation of the free energy  $P = -(\partial F/\partial V)|_T$  and the other is obtained from the relativistic virial theorem that has a uniquely useful form. In Ref. [9] we imposed equality between the two representations by adjusting the correlation energy and obtained agreement with experiments. However, this approach required assumptions on the specific form of the correction to the correlations as a functional of the local density. In the present work we bypass the specifics of the correlation energy and use a more general approach.

Explicitly we connect here the two pressure representations to obtain a differential equation for the free energy that is applicable

\* Corresponding author. 8 Lachish Street, Tel Aviv 64164, Israel.  
E-mail address: [oregi@bgu.ac.il](mailto:oregi@bgu.ac.il) (J. Oreg).

for any Coulombic neutral system. This equation determines the free energy from the lower component contribution to the electron density. Using the LDA electron density in this equation together with a proper boundary condition dramatically improves the EOS LDA results. Specifically the equation improves the LDA EOS dependence on the density while the boundary condition is employed to encompass solid structure effects that are ignored in the LDA. The model is valid over a very wide range, as will be demonstrated by various examples. In addition, it is shown that the method is applicable for mixtures.

The essentials of this approach and the notation will be given in Section 2. In this section we also describe briefly the LDA and INFERNO models as the basis of our practical calculations. In Section 3 we present the LDA virial theorem and LDA results. The differential equation for the free energy and the pressure is introduced in Section 4 where we illustrate its use to enhance the LDA results. In this section we also describe the procedure taken to use this approach for mixtures. Summary and discussion are given in Section 5.

## 2. Theoretical review

### 2.1. The relativistic virial theorem

Vast areas in physics research deal with Coulombic systems that are comprised of nuclei ( $\alpha, \beta \dots$ ) and electrons ( $i, j \dots$ ) where the potential energy operator in the Hamiltonian  $H = K + V$  is

$$V = e^2 \left[ \sum_{\alpha, \beta} \frac{Z_\alpha Z_\beta}{r_{\alpha\beta}} + \sum_{\alpha, i} \frac{Z_\alpha}{r_{i\alpha}} + \sum_{i, j} \frac{1}{r_{ij}} \right]. \quad (1)$$

The kinetic energy operators  $K$  in the Schrodinger and the Dirac theories are respectively  $K_S = -\sum_s (\hbar^2/2m_s) \Delta_s$  and,  $K_D = T_D + c^2 B$  where, in terms of the Dirac matrices  $\alpha$  and  $\beta$ ,  $T_D = c \sum_s \bar{\alpha}_s \cdot \bar{p}_s$  and  $B = \sum_s m_s (\beta - I)_s$  and  $s$  runs over all ( $i, \alpha$ ) particles.

The quantum mechanical virial theorem [9–13], which applies to all special cases (atoms, molecules, solid state, plasma etc.), can be stated as follows (for details see Appendix).

If a system contained in a volume  $V$  is Coulombic and has no external forces, the system energy in the state  $k$ , defined by  $H\psi_k = \varepsilon_k \psi_k$ , is

$$E_k = E_k(V) = \int_0^V \psi_k^* H \psi_k d\tau = \varepsilon_k N_k: N_k = N_k(V) = \int_0^V |\psi_k|^2 d\tau, \quad (2)$$

and the virial theorem reads

$$-\frac{\partial E_k}{\partial V} = \frac{1}{3V} \int_0^V \psi_k^* (T + V) \psi_k d\tau + \delta_k, \quad (3)$$

where the integrations  $\int d\tau$  is over all particles coordinates.

In Eq. (3)  $T \equiv T_S = 2K_S$  or  $T \equiv T_D = c \sum_s \bar{\alpha}_s \cdot \bar{p}_s$  in the non-relativistic or relativistic theory respectively, and  $\delta_k = S_k + \varepsilon_k (\partial N_k / \partial V)$  where

$$S_k = \int_0^V \psi_k^* H A \psi_k d\tau - \int_0^V (H \psi_k^*) A \psi_k d\tau$$

and  $A = 3V \frac{\partial}{\partial V}$  (4)

For bound states that are practically confined in  $V$ ,  $H$  is Hermitian and  $S_k = \delta_k = 0$  for any operator  $A$  yielding  $\partial E_k / \partial V = \int_0^V \psi_k^* (T + V) \psi_k d\tau = 0$ .

If, in addition, the system is subject to external forces represented by a potential  $V_{\text{ext}}$ , the resulted pressure on the system becomes

$$-\frac{\partial \bar{E}_k}{\partial V} = \frac{1}{3V} \int_0^V \psi_k^* (T + V) \psi_k d\tau + \bar{\delta}_k, \quad (5)$$

where  $\bar{E}_k = \int_0^V \psi_k^* H \psi_k d\tau$  in terms of the eigenstates  $\psi_k$  of  $H' = H + V_{\text{ext}}$  and  $\bar{\delta}_k$  depends on  $V_{\text{ext}}$ , see Appendix for details. Eq. (5) was obtained with  $\bar{\delta}_k = 0$  in several special cases [10–12] where the external forces are introduced as boundary conditions on the surface of  $V$ , or when it applies to a fully variational treatment [13a]. We will see in practical calculations that the thermal average of  $\bar{\delta}_k$  is relatively small and can be indirectly calculated. Eqs. (2)–(5) also apply in the realistic approximation where the nuclei are static. In this case the various quantities and the wave functions relate to the electrons alone and the ionic contributions are modeled and added separately.

In this work we focus on plasmas in thermal equilibrium. Eq. (5), for the electronic part, needs to be averaged over all states with their Boltzmann populations [10–13],  $f_k = \exp(-(\bar{E}_k - N\mu/kT))/U$  normalized by the partition function  $U$ , where  $N$  is the number of electrons and  $\mu$  is the chemical potential.

In the differentiation of the average energy  $E \equiv \sum_k f_k \bar{E}_k$  we use the fact that with temperature,  $T$ , as the independent variable  $-(\partial E / \partial V) = -(\partial F / \partial V)|_T$ , where  $F = E - TS$  is the free energy with the entropy  $S = -\sum_k f_k \ln f_k$ . We then obtain

$$P_F = P_V + \langle \delta \rangle_V, \quad (6)$$

where  $P_F = -(\partial F / \partial V)$  is the basic thermodynamic definition of the pressure and

$$P_V = \frac{1}{3V} \sum_k f_k \int_0^V \psi_k^* (T + V) \psi_k d\tau \equiv \frac{1}{3V} \langle T + V \rangle_V, \quad (7)$$

is the ‘virial pressure’ obtained as an expectation value with no differentiation (see Appendix). It can be easily verified that bound states, which are confined in  $V$ , do not contribute to Eq. (7). The major contributions to the pressure come from bound states that extend significantly beyond the surface of  $V$  and from semi-bound resonance states that are localized and cross beyond  $V$ . For these states, as for all continuum states that are all included in Eq. (7), the deviations from Hermiticity in  $V$  appear in  $\langle \delta \rangle_V$ . As we shall see, due to internal offsets,  $\langle \delta \rangle_V$  is relatively small and is easily incorporated, indirectly, as an adjustment to  $P_V$ .

In the Dirac theory we have the fortunate fact that only first order derivatives appear in the Hamiltonian so that in the virial theorem  $T = T_D$  with no factor 2 as in the non-relativistic case. This allows an ‘energy representation’ [9] of the virial pressure:

$$3VP_V = \sum_k f_k \langle k | T_D + V(r_i, r_{ij}) | k \rangle_V = \sum_k f_k \langle k | H_D - c^2 B | k \rangle_V, \quad (8)$$

where  $H_D = T_D + V + c^2 B$  is the Dirac Hamiltonian of the system and (in atomic units)  $B = \sum_i (\beta - I)_i = \sum_i \begin{pmatrix} \bar{0} & \bar{0} \\ \bar{0} & -2\bar{I} \end{pmatrix}_i$  where  $\bar{0}$  and  $\bar{I}$  are the  $2 \times 2$  zero and unity matrices, respectively. In this case the electronic states  $|k\rangle = \psi_k(r_1, r_2, \dots, r_N)$ , in all the equations above,

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