Energy of Quantum Coulomb Liquid

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ABSTRACT
Using Metropolis method to compute path integrals, the energy of quantum strongly-coupled Coulomb liquid (1 ≤ Γ ≤ 175) composed of distinguishable atomic nuclei and uniform incompressible electron background is calculated from first principles. The range of considered temperatures and densities represents fully-ionized layers of white dwarfs and neutron stars. In particular, the results allow one to determine reliably the heat capacity of ions in dense fluid stellar matter, which is a crucial ingredient for modelling thermal evolution of compact degenerate stars.

Key words: dense matter – stars: white dwarfs – stars: neutron.

1 INTRODUCTION
One-component plasma (OCP) is a system of identical point charges immersed into a uniform incompressible background of opposite charge to ensure overall charge-neutrality. This system is of paramount importance for astrophysics of degenerate stars, white dwarfs and neutron stars, where the point charges are bare atomic nuclei (ions) while the degenerate nearly ideal electron gas constitutes the background. For both types of stars, mass densities, at which matter can be viewed as the OCP, cannot be too low to ensure that atoms are fully ionized and electron screening is, to a good approximation, negligible. In white dwarfs, the OCP phase may extend all the way down to the center of the star (i.e. up to the highest available densities); however, several different types of atomic nuclei may be present at some densities simultaneously (e.g., C and O). Studying such multi-component plasma is beyond the scope of the present paper.

In neutron stars, matter can be treated as the OCP at least in the outer crust, i.e. all the way up to the neutron-drip density, ρd ≈ 4.3 × 1014 g cm⁻³ (with the same caveat regarding multi-ionic mixtures). It is possible that the same treatment remains valid up to higher, subnuclear, densities (in the inner crust), if the effect of dripped neutrons on the inter-ionic interaction is negligible.

Thermodynamic state of the OCP is described by just two dimensionless parameters. The Coulomb-coupling parameter Γ = Z_i^2 e^2 / (aT) measures the strength of the typical potential energy with respect to the typical kinetic energy of ions. In this case T is the temperature (k_B ≈ 1), Z_i is the ion charge number, e is the elementary charge, and a = (4πn_e/3)^{-1/3} is the ion-sphere radius (n_e is the ion number density). If one neglects the quantum aspect of the ions’ motion, Γ alone determines fully thermodynamics of the OCP. In particular, Γ = 1 signals the gas-liquid transition while Γ = Γ_m ≈ 175 corresponds to the liquid-solid transition. The strength of the ionic quantum effects is measured by the second parameter, which can be chosen as the ratio of T to the ion plasma temperature T_p = ℏ√4πnZ_i^2 e^2 / M_i, where M_i is the ion mass. In a quantum system, one has T ≪ T_p. Another often used parameter is the ratio r_s = a / a_0, where a_0 = ℏ^2 / (M_i Z_i^2 e^2) is the ion Bohr radius. These quantities are related to each other as

\[ \frac{T}{T_p} = \frac{1}{\Gamma \sqrt{\Gamma}}. \]

(1)

Thermodynamics of the OCP has been studied by many authors. In particular, the classic OCP has been studied since the 60’s (Brush, Sahlin & Teller 1966) by Monte Carlo (MC) and Molecular Dynamics (MD) methods and its thermodynamic properties are now firmly established (e.g., Slattery, Doolen & DeWitt 1982; DeWitt & Slattery 1999; Caillol 1999). The importance of the ionic quantum effects in white dwarfs (for cooling, in particular) has been appreciated since about the same time (e.g., Van Horn 1979) and was emphasized once again by Chabrier, Ashcroft & DeWitt (1992). However, there was no practical way to incorporate them. Lamb & Van Horn (1975) have constructed the first quantitative evolutionary model of white dwarfs with realistic thermodynamics but the treatment of the quantum effects was incomplete.

An important study of the quantum OCP from first principles has been conducted by Jones & Ceperley (1996). These authors used Path Integral Monte Carlo (PIMC) with 54 distinguishable particles in a simulation cell with periodic boundary conditions. For the liquid phase, they have calculated the thermal energy at Γ ≲ 160 and r_s = 100, 200, and 1200. For carbon, these r_s correspond to mass densities ρ ≈ 1.6 × 10^{13}, 2 × 10^{12}, and 10^{10} g cm^{-3}, respectively. At
such densities, carbon can hardly exist because it burns in nuclear reactions and suffers beta capture. Hence, practically important range for carbon seems to be \( r_s \gtrsim 1200 \). For heavier elements the situation is similar. For helium, it is possible to attain lower values of \( r_s \). For instance, according to table 2 of Piersanti, Tornambe & Yungelson (2014), helium may be found at \( \rho \sim 10^4 \text{ g cm}^{-3} \) (\( r_s \approx 140 \)) and \( \Gamma \sim 1 \), which, however, is not a very quantum state according to our Eq. (1). Alternatively, in table 3 of the same work, helium exists at \( \rho \sim 10^6 \text{ g cm}^{-3} \) (\( r_s \approx 650 \)) and \( \Gamma \sim 50 \), which is considerably more quantum.

In the present paper, we have decided to focus on thermodynamics of the strongly-coupled liquid regime in the range of densities \( r_s \gtrsim 600 \), where reliable quantum results are largely absent. The case of higher densities at \( \Gamma \sim 1 \) is essentially classic (but may be worth a separate study).

## 2 PATH INTEGRAL MONTE CARLO

Presently, only numerical techniques exist for first-principle studies of quantum strongly-coupled Coulomb plasma. This is true for both liquid and solid phases in which all anharmonic effects cannot be accounted for analytically. Following Jones & Ceperley (1996), we employ the PIMC method. Its detailed exposition is given in an extremely helpful review of Ceperley (1995).

In our simulation, there are \( N = 250 \) distinguishable particles (ions) placed in a cubic simulation cell with periodic boundary conditions. Each particle interacts with all periodic images of the other particles and with the uniform background. Hence, any two particles interact not via Coulomb potential, but via Ewald potential, which is a sum of Coulomb potentials of all periodic images and the background term. In this way an approximate description of an infinite system is achieved.

In order to calculate various thermodynamic averages for a quantum system, it is represented by a classical one, in which \( N \) quantum particles are replaced by \( N \) classic rings polymers with \( M \) numbered nodes ("beads") each and \( M \) links connecting beads with consecutive numbers (\( M \) is a positive integer). In each ring, there is an interaction between any two linked beads, which does not allow them to move arbitrarily far away from each other ("kinetic spring"). There is also an effective interaction between polymers originating from an interaction between beads having the same number in all rings.

If the effective interaction (known as "link action", see Ceperley 1995, for details) were known exactly, then the classical and quantum systems would be exactly isomorphic for any \( M \). However, this is not the case, and various approximations for the link action have been proposed. The simplest of them is known as the "primitive" approximation. Within its framework, the link action is directly related to the actual potential energy of \( N \) beads having the same number in their respective rings and interacting only between themselves via the Ewald potential. The primitive approximation can be shown to become exact in the \( M \to \infty \) limit.

Ceperley (1995) emphasized the utility of another approximation, the pair action, for its ability to produce correct results at smaller \( M \) than the primitive approximation in some problems (see also, Militzer & Graham 2006; Militzer 2016). A smaller \( M \) translates into less time-consuming computations. We have managed to construct the pair action for the Ewald potential including off-diagonal terms for practically relevant ranges of action arguments (not too close to zero and not too far off the diagonal). However, it has been found that the primitive approximation reproduced the zero-point energy of a Coulomb crystal (the major contribution to which is given by the well-known harmonic lattice value) at smaller \( M \) than the pair action. Consequently, we have chosen to use the primitive approximation for the action in this study.

In the primitive approximation, one needs to sample the probability distribution

\[
\pi(R_1, R_2, \ldots, R_M = R_0) = \frac{1}{Z} \exp \left[ -\sum_{m=1}^{M} S_m \right],
\]

where \( R_m \) denotes three Cartesian coordinates of all \( N \) beads with number \( m \), i.e., 750 numbers in our simulation (beads 0 are the same as beads \( M \)). Furthermore, \( Z \) is the partition function, which ensures that the distribution \( \pi \) is normalized, \( \lambda = \hbar^2/(2M\epsilon) \), \( \tau = 1/(MT) \), and \( V(R_m) \) is the potential energy of all beads number \( m \).

The sampling was done with the aid of the Metropolis algorithm. We have combined two types of moves: single bead moves using free-particle sampling and "classic" moves. In the latter we attempted to move a polymer as a whole using uniform sampling probability density within a cube whose size was chosen to ensure decent move acceptance rates. The latter moves have considerably improved the quality of our results at nearly classic \( \rho \) and \( T \).

The following quantity was used as the energy estimator (thermodynamic estimator):

\[
E = \left\langle \frac{3N}{2\tau} - \frac{(R_m - R_{m-1})^2}{4\pi \epsilon^2} + V(R_m) \right\rangle,
\]

where \( m \) is an arbitrary integer between 1 and \( M \), to which the results should not be sensitive. Angle brackets mean averaging with the probability distribution (2).

## 3 RESULTS

Thermal energy of the liquid (equal to the total internal energy minus the Madelung energy of the body-centered cubic lattice, \( E_0 \), calculated by the method described in Sec. 2, is presented in Fig. 1(a) and Table 1. Dots in Fig. 1(a) are computational results (including the extrapolation procedure below) while solid lines simply connect them to improve graph readability. We have calculated the thermal energy for 25 values of \( \Gamma \) evenly spaced between 1 and 175 (\( \Delta \Gamma = 7.25 \)) and for 15 values of \( r_s = 600, 750, 950, 1200, 1500, 1900, 2400, 3000, 3800, 4800, 6000, 8600, 15000, 30000, 120000 \). This corresponds to \( \sim 7 \) orders of density variation and, e.g., for carbon, spans the range from \( 10^4 \times 8 \times 10^{10} \) g cm\(^{-3} \) while for helium, the respective range of densities is from 0.2 to \( 10^6 \) g cm\(^{-3} \). Calculations are unreliable at the lower end of densities and such \( Z_i \), for which complete ionization is not reached, because electronic degrees of freedom
are not taken into account. Solid curves with dots correspond to different \(r_s\) with the \(r_s = 600\) curve being on top, \(r_s = 750\) the second curve from the top, \(r_s = 950\) the third, etc., and, finally, \(r_s = 120000\) is the second curve from the bottom. The (red) curve on the very bottom shows classic liquid thermal energy as calculated by Caillol (1999) and fitted by Potekhin & Chabrier (2000).

In Fig. 1(b), we compare solid curves from Fig. 1(a) for \(r_s = 600, 1500, 2400, 4800, 8600,\) and 15000 with the thermal energy of the classic liquid combined with the first quantum Wigner-Kirkwood correction (Hansen 1973) at the same \(r_s\) (dotted curves). Long dashes also include the second quantum correction of Hansen & Viellefosse (1975). The agreement with our results is quite good in a more classic range of parameters but it gets worse with increase of \(r_s\) or decrease of \(T\) (i.e., increase of \(\Gamma\)). The first quantum correction provides an adequate description of our computed values for all \(\Gamma\) in the liquid at \(r_s \gtrsim 20000\). The Hansen-Viellefosse term extends this range down to \(r_s \gtrsim 10000\). [For \(r_s = 1200\), these approximations are also plotted in Fig. 2(a).]

There are three sorts of errors that need to be addressed. Firstly, there is a systematic error stemming from the limited number of steps in the Metropolis algorithm. This error manifests itself as a dependence of energies on initial conditions, random seeds, or the number \(m\) in Eq. (3). We have analysed these dependencies for a few combinations of \(r_s\) and \(T\) and concluded that the confidence interval could be estimated at the 90% level as \(\pm 0.007\) (in absolute units) for the entire dataset. This is smaller than the dot sizes in Fig. 1(a). A much more extended computation is needed for a rigorous statistical evaluation of our data.

Secondly, there is a systematic error associated with the finite polymer size \(M\). In order to reduce this error, we have performed PIMC calculations with 4 values of \(M\): \(M_{\text{min}}\), \(2M_{\text{min}}\), \(4M_{\text{min}}\), and \(M_{\text{max}} = 8M_{\text{min}}\). For illustration, the respective energies at \(r_s = 1200\) are plotted in Fig. 2(a) by dot-dashed curves: \(M_{\text{max}}\) is the top one and all the other go progressively lower with decrease of \(M\). At each \(r_s\) and \(\Gamma\), these data have been extrapolated as functions of \(1/M\) down to \(1/M = 0\). An example of this procedure is given in Fig. 2(b) for \(r_s = 1200\) and several values of \(\Gamma\). The resulting dependence represents the exact quantum energy of 250 distinguishable particles in periodic boundary conditions. For \(r_s = 1200\), it is plotted in Fig. 2(a) by the solid line, nearly merging with the top dot-dashed line. It is this extrapolated data which are presented in Fig. 1(a) and in Table 1.

Bars in Figs. 1(a) and 2(a) represent the actual height and position of triangles from the bottom panel of fig. 3 of Jones & Ceperley (1996). We see, that at \(r_s = 1200\), our results are compatible with theirs.

Thirdly, there is a systematic error due to the finite number of particles in our simulation, \(N = 250\). In principle, a conclusive study of \(N\)-dependence must include similar calculations at several different \(N\) which is time-consuming and we defer it to a future work (see also Holzmann et al. 2016). Based on studies of smaller systems, Jones & Ceperley (1996) had come up with the following formula [their Eq. (2)]

\[
\frac{\mathcal{E}_N - \mathcal{E}_\infty}{T} = [0.035(18) - 0.0018(1)\Gamma] \frac{\Gamma}{2N},
\]

where \(\mathcal{E}_N\) and \(\mathcal{E}_\infty\) are per-particle energies in the finite system and in the thermodynamic limit, respectively, and we have taken into account that their energies were expressed in ionic Rydberg. This correction applied to \(r_s = 1200\) produces, as the \(N \to \infty\) limit, the short-dashed curve in Fig. 2(a), which barely touches the bars. Remarkably, the correction does not depend on \(r_s\) [cf. the right-hand side of Eq. (4)], and thus it will be of about the same absolute magnitude at higher \(r_s\). But this can hardly be the case, because at high \(r_s\) our numerical data are in a much better agreement with classic results plus quantum corrections, which implies that at these \(r_s\), \(N\)-correction must be negligible. In view of this controversy, we have chosen not to apply the finite \(N\) correction of Jones & Ceperley (1996) in the present work pending a detailed future study.

4 DISCUSSION AND OUTLOOK

Our results can be used to derive thermodynamic properties of matter necessary for modelling various physical phenomena in compact stellar objects.

First of all, the change of the ion energy due to quantum effects studied in the present paper, produces a change of the ion pressure and thus a slight modification of the equation of state in white dwarf cores and neutron star crusts. This effect is expected to be small though, because the total pressure is dominated by degenerate electrons.

Thermal properties of matter are modified in a more meaningful way. Consider, for instance, heat capacity. In a wide range of parameters the heat capacity is dominated by ions. This quantity is very important for a number of astrophysical applications. For one it determines cooling of white dwarfs. Reliable modelling of this process allows one to interpret observed white dwarf luminosity function and extract such a fundamental parameter as the age of the local Galactic disk (e.g., D’Antona & Mazzitelli 1990). Heat capacity of the Coulomb liquid is also needed to understand observed real-time cooling of neutron star crust heated during episodes of accretion in X-ray transients (e.g., Deibel et al. 2017), although in this case temperatures may be too high for quantum effects to be noticeable. Another promising research route is thermal evolution of accreting white dwarfs in cataclysmic variables (e.g., Gänsicke 2000).

Let us analyse two representative examples: carbon at \(\rho \approx 3 \times 10^8\) g cm\(^{-3}\) (\(r_s = 3800\)) and helium at \(\rho \approx 6.6 \times 10^5\) g cm\(^{-3}\) (\(r_s = 750\)). Ion specific heat at constant volume is

\[
\frac{C}{N} = \frac{1}{N} \left( \frac{\partial E}{\partial T} \right)_V,
\]

where \(E\) is the energy calculated in the previous section. The specific heat of carbon and helium is plotted in Fig. 3, panels (a) and (b), respectively, as a function of temperature across the melting transition. For the sake of this illustration, we have assumed that melting takes place at \(\Gamma_m = 175\). We are aware of the fact that \(\Gamma_m\) is a weak function of \(r_s\) due to quantum effects but an accurate determination of this function requires extra work and is beyond the scope of the present paper. At lower temperatures (\(T\) to the left of the discontinuities), a body-centered cubic crystal phase takes place whose specific heat is known very accurately in the harmonic approximation (Baiko, Potekhin & Yakovlev 2001).
Figure 1. (a) Calculated thermal energy of the Coulomb liquid vs $\Gamma$. From top to bottom: $r_s = 600, 750, 950, 1200, 1500, 2400, 3000, 3800, 4800, 6000, 8600, 15000, 30000, 120000$. The curve on the very bottom (red) is the classic liquid energy. Bars represent selected data points of Jones & Ceperley (1996) at $r_s = 1200$. (b) Same as in panel (a) but for $r_s = 600, 1500, 2400, 4800, 8600, 15000$ only. Dotted and long-dashed curves incorporate, respectively, the first and the second quantum Wigner-Kirkwood corrections to the classic energy.

Table 1. Numerical results for $(E - E_0)/NT$

| $r_s$ | $600$ | $750$ | $950$ | $1200$ | $1500$ | $1900$ | $2400$ | $3000$ | $3800$ | $4800$ | $6000$ | $8600$ | $15000$ | $30000$ | $120000$ |
|-------|-------|-------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|----------|-------|-----------|
| 600   | 10.364| 9.457 | 8.015 | 6.886  | 6.723  | 6.244  | 5.851  | 5.499  | 5.202  | 4.970  | 4.659  | 4.336  | 4.102  | 3.924    |
| 750   | 9.797 | 9.118 | 8.313 | 7.624  | 7.050  | 6.519  | 6.070  | 5.700  | 5.367  | 5.086  | 4.862  | 4.581  | 4.281   | 4.067   |
| 950   | 9.216 | 8.440 | 7.723 | 7.103  | 6.591  | 6.120  | 5.719  | 5.396  | 5.101  | 4.860  | 4.665  | 4.430  | 4.169   | 3.989   |
| 1200  | 8.832 | 8.103 | 7.426 | 6.864  | 6.363  | 5.920  | 5.544  | 5.234  | 4.975  | 4.763  | 4.500  | 4.226  | 3.945   | 3.781   |
| 1500  | 8.457 | 7.771 | 7.131 | 6.588  | 6.138  | 5.723  | 5.379  | 5.095  | 4.844  | 4.640  | 4.480  | 4.273  | 4.052   | 3.908   |
| 1900  | 8.080 | 7.436 | 6.838 | 6.332  | 5.913  | 5.530  | 5.210  | 4.948  | 4.718  | 4.527  | 4.379  | 4.193  | 3.997   | 3.861   |
| 2400  | 7.705 | 7.103 | 6.549 | 6.077  | 5.686  | 5.332  | 5.038  | 4.804  | 4.594  | 4.379  | 4.193  | 3.997  | 3.861   | 3.756   |
| 3000  | 7.335 | 6.775 | 6.267 | 5.826  | 5.468  | 5.143  | 4.873  | 4.655  | 4.468  | 4.310  | 4.188  | 4.038  | 3.882   | 3.769   |
| 3800  | 6.968 | 6.449 | 5.977 | 5.575  | 5.252  | 4.954  | 4.712  | 4.513  | 4.343  | 4.205  | 4.098  | 3.958  | 3.821   | 3.723   |
| 4800  | 6.599 | 6.127 | 5.698 | 5.332  | 5.038  | 4.804  | 4.594  | 4.379  | 4.193  | 3.997  | 3.861  | 3.756  | 3.626   | 3.521   |
| 6000  | 6.235 | 5.807 | 5.418 | 5.088  | 4.827  | 4.584  | 4.388  | 4.236  | 4.096  | 3.992  | 3.804  | 3.696  | 3.562   | 3.470   |
| 8600  | 5.878 | 5.492 | 5.141 | 4.848  | 4.623  | 4.405  | 4.232  | 4.098  | 3.979  | 3.885  | 3.712  | 3.633  | 3.562   | 3.470   |
| 15000 | 5.526 | 5.184 | 4.872 | 4.614  | 4.411  | 4.224  | 4.083  | 3.963  | 3.862  | 3.779  | 3.671  | 3.563  | 3.452   | 3.310   |
| 30000 | 5.176 | 4.876 | 4.607 | 4.389  | 4.215  | 4.053  | 3.930  | 3.830  | 3.749  | 3.675  | 3.622  | 3.556  | 3.494   | 3.448   |
| 120000| 4.837 | 4.578 | 4.352 | 4.165  | 4.018  | 3.885  | 3.779  | 3.698  | 3.624  | 3.569  | 3.526  | 3.471  | 3.419   | 3.384   |

It is shown by the (blue) dot-dashed curve. The (blue) short-dashed curve includes a quantum anharmonic contribution calculated in a model-dependent way by Chugunov & Baiko (2005).

In the liquid phase, we plot various approximations mentioned in Sec. 3. Upper solid curve (red) shows the specific heat of the classic liquid OCP derived from fits of Potekhin & Chabrier (2000). Dots include the first quantum correction to the classic values obtained from the Wigner-Kirkwood (WK) expansion (Hansen 1973). The long-dashed curve includes the second WK correction derived by Hansen & Viellefosse (1975). Our PIMC results are shown by the solid curve. In order to plot it, we have fitted our energy data at fixed $r_s$ by a smooth curve and differentiated it with respect to $T$.

It is interesting to observe that the specific heat jump...
Figure 2. (a) Various results at $r_s = 1200$. Four dot-dashed curves are calculations at different $M$ (curves going higher correspond to bigger $M$). Solid curve (nearly merging with the top dot-dashed curve) shows the data extrapolated to $1/M = 0$. Short-dashed curve includes the finite $N$ correction, Eq. (4). Dotted and long-dashed lines display the same Wigner-Kirkwood approximations as in Fig. 1(b). Bars represent selected data points of Jones & Ceperley (1996). (b) Extrapolation of calculated energies from finite $M$ to $1/M = 0$ at $r_s = 1200$ and five biggest values of $\Gamma$.

Figure 3. (a) Ion specific heat of carbon at $\rho \approx 3 \times 10^8$ g cm$^{-3}$. Shown are PIMC results in the liquid phase (solid curve), specific heat of the classic liquid (upper solid curve, red), first quantum correction in the liquid (dots), second quantum correction in the liquid (long dashes), harmonic lattice results in the crystal phase (dot-dashed curve, blue), quantum anharmonic correction in the crystal (short dashes, blue). (b) Same as in panel (a) but for helium at $\rho \approx 6.6 \times 10^5$ g cm$^{-3}$.

at melting (at quantum temperatures) appears to be much smaller with quantum effects included from first principles than with various approximations available previously. A more complete assessment of this result will be made when first-principle thermodynamics of the solid phase becomes available. More important, from practical point of view, is that our data indicate that the classic approximation for the specific heat can seriously overestimate it while an addition of the first WK correction yields an equally serious underestimation. The total heat capacity of a star, which determines its cooling rate, is an integral of the specific heat over the star. The degree to which the total heat capacity is affected by the quantum phenomena thus depends on the central density, temperature, and composition. A preliminary estimate suggests that in certain situations the actual heat capacity of a star may be as low as $2/3$ of the respective classic value.

Besides carbon and helium, it is just as easy to consider heavier elements. However, in order to produce quantum effects of comparable size one would have to go to much...
higher densities. Since \( r_s \) scales as \( \rho^{-1/3} Z_s^2 M_s^{4/3} \), to achieve \( r_s = 3800 \), one would require \( \rho = 5.3 \times 10^9 \) g cm\(^{-3}\) for \(^{16}\)O and \( \rho = 9.4 \times 10^{14} \) g cm\(^{-3}\) for \(^{56}\)Fe (the latter is impossible because such \( \rho \) exceeds the nuclear saturation density). In the standard picture, with growth of the mass density, lighter elements burn into heavier ones in nuclear reactions. The maximum density for a given light element to exist at a given temperature is a function of nuclear reaction rates in a strongly-coupled plasma. It is clear from the present study, that these reactions occur in the regime where quantum effects are well pronounced. Their rates are thus determined by the underlying quantum dynamics of ions and are extremely sensitive to small variations of density and temperature (e.g., Pollock \& Militzer 2004). Accordingly, it seems worthwhile to analyse the rates in detail from first principles which would require a minor modification of our code. Such a study would have implications for a wide range of astrophysical phenomena from bursts and flashes in compact stars to SN Ia.

Another thermal property, which is expected to be sensitive to quantum effects is \( \chi_T = \rho (d \ln P/d \ln T)_\gamma \) where \( P \) is the total pressure. This parameter is similar to the specific heat, Eq. (5). In both cases, one needs to differentiate a quantity dominated by degenerate electrons (energy in the case of \( C \) and pressure in the case of \( \chi_T \)). However, the differentiation is with respect to temperature which means that only thermal components of \( E \) and \( P \) really matter. This leads to a domination of ion contributions over those due to degenerate electrons. Compressibility \( \chi_T \) sets the scale of the Brunt-Väisälä frequency (e.g., Brassard et al. 1991), which, in turn, determines main properties of stellar \( g \)-modes (e.g., Montgomery \& Winget 1999). Quantum effects may change the profile of the Brunt-Väisälä frequency over a large fraction of the stellar radius. This may result in an observable change of the predicted seismological data for white dwarfs.

The present work can be also extended in other directions. An accurate energy of the solid phase can be calculated which, among other things, would allow one to determine the dependence of the latent heat of crystallization on \( r_s \) due to quantum effects. Latent heat of crystallization is another crucial parameter in the theory of white dwarf cooling. Its release delays cooling and directly affects the estimated age of a stellar population. A preliminary analysis (assuming fixed \( \Gamma_m = 175 \)) indicates that the latent heat is a weak function of \( r_s \) decreasing from \( \approx 0.77 T \) in the classic limit to \( \approx 0.71 T \) at \( r_s = 1200 \). A small correction to this dependence due to \( r_s \)-dependence of \( \Gamma_m \) is expected. Similar studies of multi-ionic mixtures can be performed with minor modifications of the same code. Finally, weak electron screening of the ion potential can be included but this will introduce an extra physical parameter into the problem.

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REFERENCES

Baiko D. A., Potekhin A. Y., and Yakovlev D. G., 2001, Phys. Rev. E, 64, 057402
Brassard P., Fontaine G., Wesemael F., Kawaler S. D., and Tassoul M., 1991, Astrophys. J., 367, 601
Brush S. G., Sahlin H. L., and Teller E., 1966, J. Chem. Phys., 45, 2102
Caillo J. M., 1999, J. Chem. Phys., 111, 6538
Ceperley D. M., 1995, Rev. Mod. Phys., 67, 279
Chabrier G., Ashcroft N. W., and DeWitt H. E., 1992, Nature, 360, 48
Chugunov A. I. and Baiko D. A., 2005, Physica A, 352, 397
D’Antona F. and Mazzitelli I., 1990, Annu. Rev. Astron. Astrophys., 28, 139
Deibel A., Cumming A., Brown E. F., and Reddy S., 2017, Astrophys. J., 839, 95
DeWitt H. E. and Slattery W. L., 1999, Contrib. Plasm. Phys., 39, 97
Gänsicke B. T., 2000, Rev. Mod. Astron., 13, 151
Hansen J. P., 1973, Phys. Rev. A, 8, 3096
Hansen J. P. and Vielufesos P., 1975, Phys. Lett. A, 53, 187
Holzmann M., Clay R. C. III, Morales M. A., Tubman N. M., Ceperley D. M., and Pierleoni C., 2016, Phys. Rev. B, 94, 035126
Jones M. D. and Ceperley D. M., 1996, Phys. Rev. Lett., 76, 4572
Lamb D. Q. and Van Horn H. M., 1975, Astrophys. J., 200, 306
Militzer B. and Graham R. L., 2006, J. Phys. Chem. Sol., 67, 2136
Militzer B., 2016, Comp. Phys. Comm., 204, 88
Montgomery M. H. and Winget D. E., 1999, Astrophys. J., 526, 976
Piersanti L., Tornambe A., and Yungelson L. R., 2014, Mon. Not. Roy. Astron. Soc., 445, 3239
Pollock E. L. and Militzer B., 2004, Phys. Rev. Lett., 92, 021101
Potekhin A. Y. and Chabrier G., 2000, Phys. Rev. E, 62, 8554
Slattery W. L., Doolen G. D., and DeWitt H. E., 1982, Phys. Rev. A, 26, 2255
Van Horn H. M., 1979, Physics Today, Jan., 23