The Rosenfeld-Tarazona expression for liquids’ specific heat: A numerical investigation of eighteen systems

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(Dated: May 9, 2013)

We investigate the accuracy of the expression of Rosenfeld and Tarazona (RT) for the excess isochoric heat capacity, $C_{V}^{ex} \propto T^{-2/5}$, for eighteen model liquids. Previous investigations have reported no unifying features of breakdown for the RT expression. Here liquids with different stoichiometric composition, molecular topology, chemical interactions, degree of undercooling, and environment are investigated. We find that the RT expression is a better approximation for liquids with strong correlations between equilibrium fluctuations of virial and potential energy, i.e., Roskilde simple liquids [Ingebrigtsen et al., Phys. Rev. X 2, 011011 (2012)]. This observation holds even for molecular liquids under severe nanoscale confinement, the physics of which is completely different from the original RT bulk hard-sphere fluid arguments. The density dependence of the specific heat is predicted from the isomorph theory for Roskilde simple liquids, which in combination with the RT expression provides a complete description of the specific heat’s density and temperature dependence.

Fundamental theories for the pressure (or density) and temperature dependence of thermodynamic quantities have gained renewed attention in the last decade. These theories can serve as a valuable input to equations of state, but also as input to scaling strategies which relate key dimensionless transport coefficients to thermodynamic quantities, such as the excess entropy (with respect to an ideal gas) or the excess isochoric heat capacity. Predicting dynamical quantities from first principles is a challenging task. One such theory is mode-coupling theory (MCT) which relates the dynamic density correlations of a fluid to its static structure. However, MCT becomes less reliable as the characterizing features of supercooled liquids become pronounced. Extensions of MCT to more complex environments, such as nanoscale confinement or homogenous shear flow, have been slow to emerge. Recently, however, other promising MCT-type-theories have started to appear for supercooled liquids.

Alternatively, theories which relate dynamics to thermodynamics such as that of Adam and Gibbs and Rosenfeld’s excess entropy scalings, relate to the dynamics also in the highly supercooled liquid regime. Excess entropy scaling strategies, as proposed by Rosenfeld, have proven succesful in predicting the dynamics of not only single-component atomic fluids, but also binary mixtures, ionic substances, small molecules, and polymers. In fact, excess entropy scaling strategies have been used as a reliable predictor even for the perplexing dynamics of nanocoﬁned liquid which exhibit stratification and position-dependent relaxation processes; the applicability of excess entropy scaling strategies to these situations emphasizes the usefulness of the thermodynamic approach to dynamics.

To fully harness the power of predicting dynamics from thermodynamics, however, it is imperative to develop reliable theories for the pressure (or density) and temperature dependence of thermodynamic quantities. Rosenfeld and Tarazona (RT) argued for a mathematically simple expression for the density and temperature dependence of the potential energy $U$ for liquids. Their arguments are based on thermodynamic perturbation theory, using the fundamental-measure reference functional for hard-spheres in combination with an expansion of the free energy around the $\eta = 1$ packing fraction. The arguments are involved and not easy to follow, but their expressions have found widespread application (Refs. 1, 2, 4, 5, 6).

From the potential energy one gains access to thermodynamic quantities such as the excess isochoric heat capacity $C_{V}^{ex} = \langle \partial U/\partial T \rangle_{V}$ and the excess entropy $S_{ex}$ via $C_{V}^{ex} = T(\partial S_{ex}/\partial T)_{V}$. Both of these quantities enter the aforementioned strategies. For a long time only few studies focused on the heat capacity. Recently, however, the heat capacity of liquids has started to receive more attention. The RT expressions for the potential energy and excess isochoric heat capacity read

$$U(\rho, T) = \alpha(\rho)T^{3/5} + \beta(\rho), \quad \text{(1)}$$

$$C_{V}^{ex}(\rho, T) = 3/5\alpha(\rho)T^{-2/5}, \quad \text{(2)}$$

where $\alpha(\rho)$ and $\beta(\rho)$ are extensive functions of density $\rho$ that relate to the specific system.

Several numerical investigations have tested the applicability of the RT expressions for various model liquids. These liquids span from simple atomic model fluids to liquids showing a wide range of structural, dynamical, and thermodynamical anomalies in their phase diagram. More specifically, the RT expressions have been investigated for single-component atomic fluids, binary mixtures, ionic substances, hydrogen-bonding liquids, small molecules, and sheared...
These investigations showed that the RT expressions give a good approximation for a range of systems, but are less accurate when applied to systems known to have strong virial/potential energy correlations, such as the Dzugutov liquid and Gaussian core model, as well as for SiO₂ and BeF₂ in their anomalous regions. For SPC/E water different results for the applicability have been reported.

The purpose of this paper is to provide insight into the conditions under which RT applies by investigating 18 different model systems possessing different stoichiometric composition, molecular topology, chemical interactions, degree of undercooling, and environment. We use GPU-optimized NVT molecular dynamics computer simulations (in total over 40000 GPU hours) to calculate the potential energy and excess isochoric heat capacity along a single isochore for each of these 18 model systems (for the single-component Lennard-Jones (SCLJ) liquid we also vary the density). Here and henceforth quantities are reported in dimensionless units, e.g., by setting σ = 1, ε = 1, etc. The heat capacity is calculated via Einstein’s fluctuation formula

\[ C_V^\text{ex} = \langle (\Delta U)^2 \rangle / k_B T^2 \]

(within statistical error, the numerical derivative of the potential energy agrees with the value calculated from the fluctuations). Previous investigations have often calculated the excess entropy, but this is computationally very demanding and not necessary to test Eqs. (1) and (2). Table I presents the investigated model systems, which range from simple atomic fluids to molecules under severe nanoscale confinement. The densities represent typical liquid-state densities.

| System                  | \( \rho \) | \( T_{\text{min}} \) | \( D_U \) | \( D_\text{ex} \) | \( R \) |
|-------------------------|-----------|----------------|--------|----------------|------|
| Core-soft water         | 0.40      | 0.138          | 0.974  | 0.473          | 0.10 |
| Dumbbell                | 0.93      | 0.380          | > 0.999| 0.999          | 0.96 |
| Nanoconfined dumbbell   | 0.93      | 0.600          | > 0.999| 0.998          | 0.91 |
| Dzugutov                | 0.80      | 0.540          | 0.997  | 0.786          | 0.71 |
| Girifalco               | 0.40      | 0.840          | 0.999  | > 0.664        | 0.91 |
| KABLJ                   | 1.20      | 0.420          | > 0.999| 0.984          | 0.93 |
| IPL 6                   | 0.85      | 0.104          | > 0.999| 0.997          | 1.00 |
| IPL 12                  | 0.85      | 0.195          | > 0.999| > 0.999        | 1.00 |
| IPL 18                  | 0.85      | 0.271          | > 0.999| 0.988          | 1.00 |
| LJC 10                  | 1.00      | 0.450          | > 0.999| 0.998          | 0.86 |
| LJC 4                   | 1.00      | 0.510          | > 0.999| 0.991          | 0.90 |
| Molten salt             | 0.37      | 0.018          | > 0.999| 0.952          | 0.15 |
| OTH                     | 0.33      | 0.640          | > 0.999| 0.995          | 0.91 |
| Repulsive LJ            | 1.00      | 0.360          | > 0.999| 0.995          | 1.00 |
| SCB                     | 1.00      | 0.960          | > 0.999| 0.991          | 0.99 |
| SCLJ                    | 0.85      | 0.700          | > 0.999| 0.974          | 0.96 |
| SCLJ                    | 0.82      | 0.660          | > 0.999| 0.962          | 0.94 |
| SCLJ                    | 0.77      | 0.740          | > 0.999| 0.940          | 0.90 |
| SCLJ                    | 0.70      | 0.860          | > 0.999| 0.954          | 0.82 |
| SCLJ                    | 0.66      | 0.910          | > 0.999| 0.959          | 0.75 |
| SCLJ                    | 0.61      | 0.980          | > 0.999| 0.859          | 0.64 |
| SCLJ                    | 0.59      | 0.990          | > 0.999| 0.729          | 0.56 |
| SCLJ                    | 0.55      | 1.050          | > 0.999| 0.644          | 0.51 |
| SPC/E water             | 1.00      | 3.800          | 0.987  | 0.558          | 0.07 |
| WABLJ                   | 1.30      | 0.670          | > 0.999| 0.911          | 0.98 |

TABLE I. Model systems investigated. \( D_U \) and \( D_\text{ex} \) are the coefficient of determination (Eq. (9)) for the potential energy and excess isochoric heat capacity, respectively, for the isochore of density \( \rho \). The virial/potential energy correlation coefficient \( R \) is given for the lowest temperature state point \( T_{\text{min}} \). The abbreviations used are: Kob-Andersen binary Lennard-Jones mixture (KABLJ); inverse power-law fluid with exponent \( n \) (IPL \( n \)); LJ polymer chain of length \( n \) (LJC \( n \)); Lewis-Wahnström \( o \)-terphenyl (OTP); single-component Buckingham liquid (SCB); single-component LJ liquid (SCLJ); Wahnström binary LJ mixture (WABLJ). The "Nanoconfined dumbbell" is confined to a (smooth) slit-pore of width \( H = 8.13 \), corresponding to roughly 16 molecular lengths.

Figures (a) and (b) show, respectively, the potential energy and excess isochoric heat capacity at constant density as a function of temperature for all investigated systems. In all cases, the excess isochoric heat capacity decreases with increasing temperature.
model systems. (a) The potential energy

\[ U \] per atom as a function of temperature (the values for SPC/E water have been shifted for clarity with -3 in the x-direction). For all liquids, bonding or strongly ionic or dipolar liquids are generally not expected. For many of the investigated systems that fall into this simple class such a correlation is not expected from the original RT bulk hard-sphere fluid derivation (see below). The latter reflects the fact that directional or competing interactions tend to destroy the strong virial/potential energy correlation.

Turning now to the RT expressions, we show in Figs. 2 a) and (b) the coefficient of determination \( D \) for the potential energy and excess isochoric heat capacity as a function of \( 1 - R \) (see below). For a generic quantity \( X \), the coefficient of determination \( D_X \) is defined by

\[
D_X = 1 - \frac{\sum_{i=1}^{N} (X_i - f(X_i))^2}{\sum_{i=1}^{N} (X_i - \langle X \rangle)^2},
\]

where \( f(X_i) \) is a function that provides the model values, and the average \( \langle X \rangle \) is taken over a set of data points \( X = \{X_1, ..., X_N\} \). In our case \( f(X_i) \) is given by fits to the data points in \( X \) using, respectively, \( U = A_0 T^{3/5} + A_1 \), and \( C_V^{\text{ex}} = 3/5 A_2 T^{-2/5} \), where \( A_0, A_1, \) and \( A_2 \) are constants. \( D_X \) measures the proportion of variability in a data set that is accounted for by the statistical model; \( D_X = 1 \) implies perfect account of the variability.

The virial/potential energy correlation coefficient \( R \) is defined via

\[
R = \frac{\langle DW DU \rangle}{\sqrt{\langle (DW)^2 \rangle} \sqrt{\langle (DU)^2 \rangle}},
\]

and calculated from the canonical ensemble equilibrium fluctuations at \( T_{\min} \). A new class of liquids was recently proposed, namely the class of strongly correlating liquids. These liquids are simple in the Roskilde sense of the term and defined by \( R \geq 0.90 \). Only inverse power-law fluids are perfectly correlating (\( R = 1 \)), but many models as well as experimental liquids have been shown to belong to the class of Roskilde simple liquids. This class is believed to include most or all van der Waals and metallic liquids, whereas covalently, hydrogen-bonding or strongly ionic or dipolar liquids are generally not Roskilde simple. The latter reflects the fact that directional or competing interactions tend to destroy the strong virial/potential energy correlation.

By plotting \( D \) as function of \( 1 - R \), we investigate whether a correlation between the "simple" expression of RT for the specific heat and "Roskilde simple liquids" exists. For many of the investigated systems that fall into this simple class such a correlation is not expected from the original RT bulk hard-sphere fluid derivation (see below).
Roskilde simple single-component atomic systems implies this behavior.

We have shown that the key determining factor for RT is not whether systems are atomic or molecular (see results for dumbbell, OTP, and LJC), but rather the degree of strong correlation between virial and potential energy. This was shown to be the case even for severely nanoconfined molecular systems which exhibit a completely different physics from bulk hard-sphere fluids and are thus not expected to satisfy the original RT arguments. The latter is, in particular, true also for the elongated non-spherical molecules studied here. The observed correlation between RT and Roskilde simple liquids is thus highly nontrivial.

As a further validation of the above viewpoint, we relate the function $\alpha(\rho)$ in the RT expression to $h(\rho)$ for Roskilde simple liquids. For such a liquid, temperature separates into a product of a function of excess entropy per particle and a function of density via $T = f(s_{ex})h(\rho)$. Roskilde simple liquids are characterized by having isomorphs to a good approximation. Isomorphs are curves in the thermodynamic phase diagram along which structure and dynamics in reduced units, as well as some thermodynamic quantities are invariant. Along an isomorph both $C_V^{ex}$ and $h(\rho)/T$ are invariant, and consequently one may write

$$C_V^{ex} = F\left(\frac{h(\rho)}{T}\right).$$

Since by the RT expression; $C_V^{ex} = 3/5\alpha(\rho)T^{-2/5} = 3/5(\alpha(\rho)^{5/2}/T)^{2/5}$, it follows that $h(\rho) = \alpha(\rho)^{5/2}$ or, equivalently,

$$\alpha(\rho) = h(\rho)^{2/5}. \quad (6)$$

For a LJ system, it was shown in Refs.27 and 86 that $h(\rho)$ is given by

$$h(\rho) = (\gamma_0/2 - 1)\rho^4 + (2 - \gamma_0/2)\rho^2, \quad (7)$$

in which $\gamma_0$ is calculated from the virial/potential energy fluctuations at $\rho = 1$ and $T = 1$ via $\gamma_0 = \langle\Delta W/\Delta U\rangle/(\langle\Delta U\rangle)^2$.

Equation (6) is tested in Fig. 3 for the KABLJ and the repulsive LJ system (for which, respectively, $\gamma_0 = 5.35$ and $\gamma_0 = 3.56$). The repulsive LJ system is defined from $v(r) = (r^{-12} + r^{-6})/2$ and has $R$ above 99.9% in its entire phase diagram; $\gamma$ varies from 2 at low density to 4 at high density. We determine $\alpha(\rho)$ for different densities by fitting Eq. (4) as a function of temperature for each isochore and system. $h(\rho)$ is calculated analytically from Eq. (4). Figure 3 shows that $\alpha(\rho)$ as predicted by the isomorph theory to a very good approximation is given by $h(\rho)^{2/5}$. A complete description is thus given via Eqs.
Scaling strategies which relate dynamics to thermodynamics have in the past proven useful to predict perplexing dynamical phenomena. We identified here the range of applicability for RT as the class of Roskilde simple liquids. By combining the RT expressions with the isomorph theory, we were able to provide also the full density and temperature dependence of the specific heat, i.e., $C_V^\text{CS} = (h(\rho)/T)^{2/5}$.

The predictive power of the aforementioned scaling strategies for most van der Waals and metallic liquids is hereby significantly increased.

FIG. 3. $\alpha(\rho)$ in the RT expression plotted as a function of $h(\rho)$ of the isomorph theory (Eq. (4)) for the KABLJ and repulsive LJ system (see text). The red and blue curves are proportional to $h(\rho)^{2/5}$ with the proportionality constant determined from the highest density state point ($\rho = 4.00$) for each system.

The center for viscous liquid dynamics "Glass and Time" is sponsored by the Danish National Research Foundation via Grant No. DNRF61. We thank Lasse Bøhling for providing some of the data that establish the background for Fig. 3. Useful discussions with Truls Ingebrigtsen and Jacob Marott are gratefully acknowledged.

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