The efficacy of isotope thermometry: examining in the S-matrix approach

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Isotope thermometry, widely used to measure the temperature of a hot nuclear system formed in energetic nuclear collisions, is examined in the light of S-matrix approach to the nuclear equation of state of disassembled nuclear matter. Scattering between produced light fragment pairs, hitherto neglected, is seen to have an important bearing on the extraction of system temperature and volume at freeze-out from isotope thermometry. Taking due care of the scattering effects and decay of the primary fragments, a more reliable way to extract the nuclear thermodynamic parameters is suggested by exploiting least-squares fit to the observed fragment multiplicities.

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Theoretical investigations on the equation of state (EOS) of infinite [1, 2, 3, 4] and finite [2, 4, 5, 6, 8, 9, 10] nuclear matter predict the existence of a liquid-gas (LG) type phase transition in these systems. This transition is thought to play an important role in nucleosynthesis in supernova explosion [11, 12]. Laboratory experiments in collisions between energetic nuclei appear to reveal signals of LG phase transition in hot finite nuclear systems [13, 14, 15]. Proper identification of such a transition, however, depends on the reliable measurement of the thermodynamic observables. In particular, temperature plays a pivotal role. An widely used practice to extract the temperature of hot nuclear systems is to take resort to double-isotope ratio thermometry as suggested by Albergo et al. [16]. In an ideal scenario, the primary fragments produced in the freeze-out volume are assumed to be in their ground states. Particle and γ-decay corrections to the excited primary fragments have also been built in [17]. Generally, the feeding effect of secondary decay has been accounted through a correction factor [13, 14, 19, 20] on the measured multiplicities. The temperature is seen to increase by ∼ 10-20 % from the ideal situation.

All these analyzes have been done with the assumption that the fragment species produced are noninteracting within the freeze-out volume. Strong interaction corrections, appropriately taken up in the S-matrix approach [21] to the grand partition function of the dilute nuclear system, where in addition to all the stable mass particles, the two-body scattering channels between them can be included systematically are seen to modify the fragment multiplicities [22, 23]. The extracted temperature as obtained in the previous analyses without strong interaction corrections may then differ from the real temperature at which the fragments were produced. In a schematic calculation [24] in S-matrix approach in dilute infinite nuclear matter, neglecting secondary decay, we found that the scattering effects on the extracted temperature and volumes are not negligible. In the present communication, these ideas are incorporated to provide a realistic framework to analyze the data in an experimental multifragmentation set up to extract the temperature and volume of a finite disassembling nucleus at freeze-out with explicit inclusion of γ and particle decay as well as effects from scattering between different fragment species.

The details of the S-matrix approach, as applied to nuclear systems, are given in Refs. [22, 24, 25]. For completeness, a few relevant equations are presented here highlighting the approximations. The grand partition function $\mathcal{Z}$ of a system in thermodynamic equilibrium can be written as a sum of three terms [21]:

$$\ln \mathcal{Z} = \ln \mathcal{Z}_{gr} + \ln \mathcal{Z}_{ex}^0 + \ln \mathcal{Z}_{sc}.$$  \hspace{1cm} (1)

The first and second terms correspond to the contributions from the ground states and particle-stable excited states of all the produced fragment species behaving like an ideal quantum gas. The last term sums up the contributions from the scattering states, expressible in terms of the S-matrix elements. Formal expressions for these three terms are spelt out in Ref. [23].

The scattering channels, for convenience, can be separated into two parts, one containing only light particles and the other the heavy ones, i.e.,

$$\ln \mathcal{Z}_{sc} = \ln \mathcal{Z}_{sc}^l + \ln \mathcal{Z}_{sc}^h.$$  \hspace{1cm} (2)

The scattering of the heavy ones is dominated by a multitude of resonances near the threshold; the S-matrix elements can then be approximated by resonances, which...
like the excited states are again treated as ideal gas terms \[29\]. These are the particle-unstable states. Structurally, in \(Z_{sc}^i\) being then similar to \(\ln Z_{sc}^0\) \(\ln Z_{ex}^0\) and \(\ln Z_{ex}^h\) are combined together to give in \(Z_{ex}^i\) \((= \ln Z_{ex}^0 + \ln Z_{ex}^h)\), which contains contributions from particle-unstable excited states besides the particle-stable ones.

In \(\ln Z_{sc}^i\), only the elastic scattering channels for the pairs \(NN, Nt, N^3He, N\alpha\) \((N\alpha\) refers to the nucleon) and \(\alpha\alpha\) have been included. These calculations involve virial coefficients \[23, 27\] that are functions of only experimental entities, namely, phase shifts and binding energies. Once the partition function is obtained, total fragment multiplicities \(Y_i\) for the \(i\)-th fragment species with \(N_i\) neutrons and \(Z_i\) protons can be evaluated as

\[Y_i = \zeta_i \left( \frac{\partial}{\partial \zeta_i} \ln Z \right)_{V,T}. \tag{3}\]

Here \(\zeta_i \equiv \zeta_{N_i,N_i}\) is the effective fugacity defined as \(\zeta_{N_i,N_i} = e^{\beta (\mu_{N_i} + B(A_i, Z_i))}\) \(B(A_i, Z_i)\) is the binding energy of the fragment and \(\mu_{N_i, N_i}\) is its chemical potential, which from chemical equilibrium is \(\mu_{N_i, N_i} = N_i \mu_n + Z_i \mu_p\), \(\mu_n\) and \(\mu_p\) being the neutron and proton chemical potentials obtained from the conservation of the total neutron and proton numbers of the system, \(\beta\) is the inverse temperature.

For relatively low density and not too low temperature, assuming that the quantum distribution can be replaced by a classical one, expressions for the primary fragment multiplicities of the \(i\)-th species can be derived as follows.

\[Y_i = V A_i^{3/2} \sum_{j} \gamma_j e^{-\gamma_j/T} + Y_{sc}^i. \tag{4}\]

In Eq. (4), \(V\) is the volume of the system, \(\lambda = \sqrt{2\pi/mT}\) (we use natural units \(\hbar = c = 1\)) is the nuclear thermal wavelength and \(g_0^i\) and \(g_j^i\) are the degeneracies of the ground and excited states. The sum over the excited states includes both \(\gamma\) and particle-decay (resonance) channels. In different variants of the models of nuclear statistical equilibrium, only the first term (that also implicitly contains scattering corrections from resonances in heavy fragments) on the right hand side of Eq. (4) has been used to obtain the nuclear thermodynamic observables. The last term \(Y_{sc}^i\) is the contribution to the fragment yield from scattering, it is nonzero only for the fragments in the light species set. Expressions for the multiplicity yields \(Y_{sc}^0, Y_{sc}^h\) etc. (collectively written as \(Y_{sc}^i\)) are given in Ref. \[22\]. From now on, corrections obtained with the use of \(Y_{sc}^i\), in the extraction of nuclear parameters would be called scattering corrections.

The multiplicities of the primary excited fragments as obtained in Eq. (4) undergo changes because of subsequent particle emission. The secondary yield can be written in terms of the variables \(V, \mu_n, \mu_p\) and \(T\) at freeze-out as follows. For light fragments \((A_i \leq 4, Z_i \leq 2)\),

\[Y_i(A_i, Z_i) = V g_0^i A_i^{3/2} e^{\beta (N_i \mu_n + Z_i \mu_p + B(A_i, Z_i))/T} + \]

\[V \sum_j \sum_k \left( \frac{A_i^{3/2}}{A^3} e^{\beta (N_j \mu_n + Z_j \mu_p + B(A_j, Z_j))/T} \right) \times \omega_{kp}^i(A_j, Z_j, T) x_{kj}(A_j, Z_j, T) \}

\[\left(\{\text{all } \gamma\} + Y_{sc}^i, \right) + Y_{sc}^i. \tag{5}\]

The light fragments are assumed to be produced only in their ground states, their multiplicities being given by the sum of the first and the last terms in Eq. (5). Their population is further fed from decay of heavier species given by the second term. The sum \(j\) runs over all species with \(A_j > 4\) and \(Z_j > 2\) having particle-unstable excited states and the sum \(k\) runs over all the particle-decaying states of the \(j\)-th species. The quantity \(x_{kj}\) corresponds to the branching ratio of the \(k\)-th state for emitting the \(i\)-th species; it is calculated using the Weisskopf-Ewing model \[28\]. The quantity \(\omega_{kp}^i\) is the internal partition function for the particle-unstable states

\[\omega_{kp}^i(A_j, Z_j, T) = g_k e^{-\gamma_k/T}. \tag{6}\]

For heavy particles \((A > 4, Z \geq 2)\), the observed yield is

\[Y(A, Z) = V A^{3/2} e^{\beta (N_\mu + Z \mu_p + B(A, Z))/T} \times \left\{ g_0(A) + \omega_{\gamma}(A, Z, T) \right\} \]

\[+ \sum_{i=1}^6 \sum_{k,j=1}^6 \left( \frac{A_i}{A} \right)^{3/2} e^{\beta (n_i \mu_n + z_i \mu_p + B(A + a_i, Z + z_i) - B(A))/T} \times \omega_{kp}^i(A + a_i, Z + z_i, T) x_{kj}(A + a_i, Z + z_i, T) \}

\[\left(\{\text{all } \gamma\} + Y_{sc}^i, \right) + Y_{sc}^i. \tag{7}\]

In Eq. (7), \(\omega_{\gamma} \equiv \sum_k g_k e^{-\gamma_k/T}\) is the partition function for \(\gamma\)-decaying states, the sum \(i\) runs over the emitted ejectiles for which we take only \(n, p, d, t, ^3\)He and \(\alpha, a_i, z_i\) being their mass and charge. Kolomiets et al. \[17\] arrived also at expressions of the type given in Eqs. (5) and (7), the important difference being the absence of the scattering correction and consideration of only the dominant decay mode. They further considered only nucleon and \(\alpha\)-decay channels. Moreover, the feeding to the light fragment yield was neglected. Given a set of experimental yields for four fragments, their single ratios are obtained at expressions of the type given in Eqs. (5) and (7) resulting in a system of three independent equations. The equations are solved iteratively in Newton-Raphson method yielding values of \(\mu_n, \mu_p\) and \(T\). The volume can then be determined knowing the yield of a fragment.

To explore the effect of scattering on the extracted values of \(T\) and \(V\) of a hot fragmenting system, we take resort to a numerical experiment. The primary fragment yields are calculated with given freeze-out temperature \(T_{fz}\) and volume \(V_{fz}\) in the S-matrix approach as elucidated. The secondary yields are then calculated using Eqs. (5) and (7). These are taken as observed numerical data. In Eq. (7), the first term in the
by the last term in Eq. (5). One has to further consider scattering corrections as given taken \[30, 31\] into consideration. For still heavier nuclei, as well as their decay modes for \(5 \leq A \leq 16\) have been taken \[30, 31\] into consideration. For still heavier nuclei, the sum over excited states in Eqs. (5) and (7) is replaced by an integral convoluted with the single-particle level density \(\omega(A, E)\) \[23, 32\]. The integration limits are taken between 2 MeV (approximated for the first excited state) and 8 MeV (the last particle-stable state) for the \(\gamma\)-decaying levels; the resonance limit is taken as 20 MeV. The calculations done at different temperatures in a freeze-out volume \(4V_0\) \(V_0\) is the normal volume of \(^{124}\text{Sn}\) have been chosen. We have chosen two sets of four fragments, namely, \(^3\text{He}, ^4\text{He}, ^6\text{Li}, ^7\text{Li}\) and \(^3\text{He}, ^4\text{He}, ^{10}\text{Be}, ^{11}\text{Be}\) which we refer to as \(\text{He-Li}\) and \(\text{He-Be}\) thermometers. The extracted apparent temperatures \(T_{app}\) are found to be quite sensitive to the different approxima-
tions as displayed in the left panels of Fig. 1. Except for \(T_{alb}\), the other temperatures are not very sensitive to the choice of thermometer. Successive improvement of approximations is seen to bring the apparent temperature closer to the real one. With inclusion of effects due to \((\gamma + p)\)-decay and scattering, the apparent temperature \(T_{\gamma+p+sc}\) when calculated yields the actual temperature \(T_{fz}\). The effect of scattering is seen to be substantial.

The volume \(V_{app}\) (measured in units of \(V_{fz}\)) extracted in different approximations is displayed in the left panels of Fig. 2 as a function of \(V_{fz}\) for the above mentioned thermometers. Scattering has a comparatively more significant role here than that observed in the determination of temperature. Its inclusion collapses the apparent volumes \(V_{app}/V_{fz}\) to unity.

The method so discussed suffers from two limitations. For many thermometers, there may not be convergence for the solution as noted earlier \[17\]. We also found that there may be multiple solutions. We have presented those solutions that are robust in the sense that taking a considerable range of initial guess values in the iterative method, same solutions are obtained. To overcome these limitations, we propose that the least-squares fit to the secondary multiplicities may be more fruitful in extracting the temperature and volume. Given experimental yields for a chosen number of fragment species \(n_{iso}\), the least-squares fit to

\[
\sum_{i=1}^{n_{iso}} [Y_i^{exp} - Y_i(T, V, \mu_n, \mu_p)]^2 = \chi^2
\]

has been performed. The quantities \(Y_i^{exp}\) are the experimental multiplicities which are functions of the thermodynamic variables at freeze-out and \(Y_i(T, V, \mu_n, \mu_p)\) are

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{In panels (a) and (b), the extracted temperature \(T_{app}\) for the fragmenting system \(^{124}\text{Sn}\) as a function of the freeze-out temperature \(T_{fz}\) shown for two different thermometers under different approximations using single ratios (SR). In panels (c) and (d) the same are shown using least-squares method (LS) for two sets of isotopes as mentioned in the text. The dashed-dot, dotted, dashed and full lines correspond to \(T_{alb}, T_\gamma, T_{\gamma+p}\) and \(T_{\gamma+p+sc} = T_{fz}\), respectively.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig2}
\caption{The same as in Fig. 1 for the extracted volume \(V_{app}\) in units of freeze-out volume \(V_{fz}\).}
\end{figure}
the yields calculated from Eqs. (5) and (7) with various approximations as explained earlier. In our calculations, $V_{n,app}$ are taken from our numerical experiment. The extracted temperatures $T_{app}$ in the least-squares method for the system $^{124}$Sn at different given $T_{fz}$ and at a freeze-out volume $V_{fz} = 4V_0$ under different approximations are displayed in the right panels of Fig. 1. The calculations have been performed using a set of light isotopes with $n_{iso} = 6$ ($n, p, d, t, ^3$He and $^4$He). The calculations are repeated with a broader set ($n_{iso}=13$) that includes, besides the light set also the nuclei $^6$Li, $^7$Li, $^9$Be, $^{10}$B, $^{12}$C, $^{14}$N and $^{16}$O. The $\gamma$-decay corrected temperature $T_\gamma$ is found to be insensitive to the choice of fragment set and underestimates $T_{fz} (= T_{\gamma+p+\beta})$ considerably. Inclusion of particle-decay narrows the gap from $T_{fz}$ significantly, particularly for the broader set of fragment species. Right panels of Fig. 2 display the extracted volume $V_{app}$ as a function of the freeze-out temperature. The $\gamma$-decay corrected volume $V_\gamma$ overestimates $V_{fz}$ significantly. Inclusion of particle-decay brings it closer to $V_{fz}$, particularly for the larger set. The uncertainty in the ($\gamma+p$)-corrected value for the volume, with $n_{iso}=13$, is seen to be at most 25% and that for temperature, it is at most 5%. Inclusion of heavier species in the fitting procedure masks the scattering effects. The calculations have been repeated for $V_{fz}=6V_0$ and $8V_0$; the conclusions do not change for this range of freeze-out volumes.

Along with temperature and volume, the nucleon chemical potentials $\mu_n$ and $\mu_p$ are also extracted in this method which are not shown here. With the knowledge of these four thermodynamic parameters, it is straightforward to determine the entropy of the disassembling system. Thus the evolution of entropy with $T_{fz}$ can be known which acts as an important signature for the liquid-gas type phase transition. This will be reported elsewhere.

In this paper, limitations of the currently used isotope thermometry to determine the temperature and volume of a hot fragmenting nuclear system has been pointed out. It is stressed that the strong interaction effects left out in such a determination leaves a sizeable uncertainty. This has an important bearing on many predictions on the properties of hot finite nuclear matter. A new method, namely the least-squares fit to the fragment multiplicities is proposed to extract the thermodynamic observables. We find this more promising in a numerical experiment, this can be readily implemented in a realistic experimental situation.

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