Influence of the Coulomb Interaction on the Chemical Equilibrium of Nuclear Systems at Break-Up

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Abstract

The importance of a Coulomb correction to the formalism proposed by Albergo et al. for determining the temperatures of nuclear systems at break-up and the densities of free nucleon gases is discussed. While the proposed correction has no effect on the temperatures extracted based on double isotope ratios, it becomes non-negligible when such temperatures or densities of free nucleon gases are extracted based on multiplicities of heavier fragments of different atomic numbers.

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The formalism by Albergo, Costa, Costanzo, and Rubbino (ACCR) offers simple and elegant prescriptions for the experimental determination of the temperature $T$, and of the free nucleon densities, $\rho_{nF}$ and $\rho_{pF}$ in a nuclear system at the instance of the break-up. This formalism presumes a specific scenario for the decay of excited systems, similar to the scenarios modeled by the Berlin Microcanonical Metropolis Monte Carlo and the Copenhagen Statistical Multifragmentation models. Therefore, it may be expected to be meaningful in circumstances (in an excitation energy domain), where the use of the above two more complete models can be justified. On the other hand, the ACCR formalism is incompatible with models such as the equilibrium-statistical model GEMINI and the
Expanding Emitting Source Model [3], both of which refer to sequential decay scenarios of systems of uniform density. The purpose of the present paper is to point out that in certain circumstances, the approximation of the free nucleon gas as a collection of non-interacting nucleons, as assumed in the original ACCR approach, may not be sufficiently accurate, and that the inclusion of a proper Coulomb correction term is warranted. Regardless of the magnitude of the effects of such a correction, its inclusion is warranted already by didactical considerations.

The ACCR formalism [1] refers to a fragment production scenario in which an equilibrated freeze-out/break-up configuration emerges from initial compression and expansion stages. In this formalism, the average numbers of fragments or clusters of different mass and atomic numbers \((A, Z)\) are determined by the requirement of chemical equilibrium between the fragments and free nucleons - neutrons and protons (quite obviously, the fragments are then also in a state of chemical equilibrium among themselves). In Ref. 1, the chemical equilibrium between fragments \((A, Z)\) and gases of free neutrons and free protons is described by the equation

\[
\tilde{\mu}_{A,Z} - B_{A,Z} = Z\tilde{\mu}_{pF} + (A - Z)\tilde{\mu}_{nF},
\]

where \(B_{A,Z}\) is the fragment binding energy (taken with positive sign) and \(\tilde{\mu}_{A,Z}, \tilde{\mu}_{nF},\) and \(\tilde{\mu}_{pF}\) are the reduced chemical potentials of a fragment \((A, Z)\), of a free neutron, and a free proton, respectively. Here, the qualifier “reduced” is used with respect to the term chemical potential and a tilda is used in the respective symbolic representation, to distinguish the quantities involved in Eq. [1] from the true thermodynamical chemical potentials \(\mu_{A,Z}\), as defined via the equation

\[
\mu_{A,Z} = \left[ \frac{\partial F(V,T)}{\partial N_{A,Z}} \right]_{V,T}.
\]

In Eq. [2], \(F(V,T)\) is the free energy of the system at volume \(V\) and temperature \(T\). The quantity \(N_{A,Z}\) is the average number of fragments \((A, Z)\), and the partial derivative is taken at constant temperature and volume. Note that, unlike their “reduced” counterparts \(\tilde{\mu}_{A,Z}\),
the true chemical potentials $\mu_{A,Z}$ include not only the binding energy term $B_{A,Z}$, but also the energy of interaction of the fragments $(A, Z)$ with the relevant mean Coulomb field. When true chemical potentials are considered, the chemical equilibrium is expressed through the following equation:

$$
\mu_{A,Z} = Z\mu_{pF} + (A - Z)\mu_{nF} - V_{\text{coul}}^{pF}(Z),
$$

(3)

where $V_{\text{coul}}^{pF}(Z)$ is the average energy of mutual Coulomb interaction of $Z$ free protons. The latter Coulomb interaction energy must be subtracted on the right-hand side of Eq. 3 to compensate for the fact, that in a mean-field type of “bookkeeping” of the Coulomb energy that is included in the term $Z\mu_{pF}$, the mutual Coulomb interaction energy is double-counted.

For some purposes, one may consider the convenient notion of a reduced chemical potential $\tilde{\mu}(A, Z)$, which excludes the fragment binding energies and the interaction with the mean Coulomb field. In Maxwell-Boltzmann statistics, the latter quantity has a simple relationship \cite{1} to the density $\rho_{A,Z}$ of fragments $(A, Z)$ representing the number of fragments per unit break-up volume:

$$
\rho_{A,Z} = \frac{A^2\omega_{A,Z}(T)}{\lambda_T^3}e^{\tilde{\mu}_{A,Z}/T}.
$$

(4)

Eqs. 3 and Eq. 4 are the two fundamental equations used in Ref. \cite{1} to establish the relationship between the yields of various fragments and the characteristics of a chemically equilibrated nuclear system at break-up. In Eq. 4, $\lambda_T = \hbar/\sqrt{2\pi m_o T}$ is the nucleon thermal wave-length ($m_o$ is the mass of a nucleon), and $\omega_{A,Z}(T)$ is the temperature-dependent internal partition function of fragment $(A, Z)$:

$$
\omega_{A,Z}(T) = \sum_k (2s_k^{A,Z} + 1)e^{-E_k^{A,Z}/T},
$$

(5)

where the summation extends over all bound states of the fragment $(A, Z)$ with spins $s_k^{A,Z}$ and excitation energies $E_k^{A,Z}$.

An inspection and comparison of Eq. 3 to the more fundamental Eq. 3 reveals a lack of symmetry of the former equation. While the fragment $(A, Z)$ side of the balance includes
the mutual interaction energy of the constituent nucleons - the binding energy \( B_{A,Z} \), no equivalent term is present for the free nucleons on the r.h.s. of Eq. 1. Yet, the \( Z \) free protons do interact among themselves via long-range Coulomb interactions. Therefore, a more complete equation for the chemical equilibrium based on Eq. 3 must include the respective Coulomb interaction term. Note that, on the fragment side of the balance, the mutual Coulomb interaction energy of \( Z \) protons is included in the binding energy term \( B_{A,Z} \). One may note also that neither side of Eq. 1 considers explicitly (or implicitly) the Coulomb interaction energy of the \( Z \) protons with the remaining \( (Z_{\text{system}} - Z) \) “spectator” protons of the system. Such an omission, however, may be well justified, as these two Coulomb interaction energies are to a good approximation equal to each other and, hence, cancel mutually.

A more complete, Coulomb-corrected equation for the chemical equilibrium of fragments \((A, Z)\) and free nucleons, in terms of reduced chemical potentials \( \tilde{\mu}_{A,Z} \) has the symmetrical form:

\[
\tilde{\mu}_{A,Z} - B_{A,Z} = Z \tilde{\mu}_{pF} + (A - Z) \tilde{\mu}_{nF} + V_{pF}^{\text{coul}}(Z). \tag{6}
\]

Here, \( V_{pF}^{\text{coul}}(Z) \) represents the average potential energy of the mutual Coulomb interaction of \( Z \) free protons, an equivalent of the term \(-B_{A,Z}\). It is worth noting that, here (unlike in Eq. 3) the Coulomb interaction term enters with positive sign, as no Coulomb interaction is included in the reduced free-proton chemical potential \( \tilde{\mu}_{pF} \).

While it is clear from simple estimates that the Coulomb correction term, \( V_{pF}^{\text{coul}}(Z) \), is of non-negligible magnitude when compared to typical temperatures of the system, it is not obvious how to actually evaluate it. A conservative estimate for the value of \( V_{pF}^{\text{coul}}(Z) \) may be obtained by assuming that this term is equal to the Coulomb interaction energy of \( Z \) protons uniformly distributed over a spherical volume \( V_{\text{free}} = Z / \rho_{pF} \), i.e., distributed with a density equal to that of the gas of free protons \( \rho_{pF} \) at break-up. In this case, the correction term is independent of the fragment mass number \( A \):
\[ V_{\text{coul}}^p(Z) = \frac{3}{5} \frac{e^2 Z^2}{(\frac{3Z}{4\pi \rho_p})^{1/3}} \approx 1.39 Z^{5/3} \rho_p^{1/3} (\text{MeV}), \]  

(7)

where \( \rho_p \) is expressed in units of \( fm^{-3} \).

The presence of the Coulomb correction term \( V_{\text{coul}}^p(Z) \) in Eq. 6 modifies the basic equation 5 of Ref. [1] for the average number of fragments \((A, Z)\) per unit break-up volume, \( \rho_{A,Z} \). It can now be written more accurately as

\[
\rho_{A,Z} = \frac{A^{3/2} \lambda_T^{A-1} \omega_{A,Z}(T)}{2A} \rho_p Z A^{-Z} e^{[B_{A,Z} + V_{\text{coul}}^p(Z)]/T},
\]

(8)

replacing Eq. 4. In Eq. 8, \( \rho_n \) and \( \rho_p \) are the densities (i.e., numbers per unit break-up volume) of free neutrons and free protons, respectively. A similar result was obtained earlier based on a more rigorous macrocanonical description of a decaying nuclear system in a freeze-out configuration. It is worth noting that, in more complete theoretical descriptions of equilibrated freeze-out configurations, offered by the Berlin and Copenhagen models, the effects of the Coulomb interaction of the free protons are accounted for in a rigorous fashion, but remain largely transparent to the model users.

In practical applications of Eq. 8, ratios of properly selected densities, \( \rho_{A_1,Z_1}/\rho_{A_2,Z_2} \), are taken and identified with the ratios of the respective experimental yields of fragments \( Y_{A_1,Z_1}/Y_{A_2,Z_2} \). Such ratios are free of some model parameters (e.g., of the densities of free neutron and proton gases, in the case of double isotope ratios), providing often a simple link between observable yields and selected characteristics of the break-up state.

It is clear from Eq. 8 that the introduction of the Coulomb correction term \( V_{\text{coul}}^p(Z) \) is of no consequence when ratios of yields are taken for fragments with identical atomic numbers \( Z \), i.e., ratios of experimental fragment yields of the type \( Y_{A+1,Z}/Y_{A,Z} \). In such cases, the corresponding Coulomb correction terms for the two isotopes involved cancel each other. As a result, this correction has no effect on the outcome of an experimental evaluation of break-up temperatures based on double-isotope ratios - the most common use of the ACCR approach. A similar cancellation does not, however, occur in cases when, e.g., an experimental “thermometer” is constructed from isotope ratios, \( Y_{A+1,Z+1}/Y_{A,Z} \), or in cases...
when relative densities of free neutron and proton gases, $\rho_{nF}/\rho_{pF}$, are determined based on an isobaric ratio $Y_{A,Z}/Y_{A,Z+1}$. To assess the significance of the proposed Coulomb correction, several examples are considered below. In these examples, it is assumed that $T=3.3$ MeV (as found [7] for the system S+Ag at $E/A=22$ MeV) and $\rho_{pF} = 5/(4/3\pi 8.0 \times 141) = 0.0011$ fm$^{-3}$ (which corresponds to 5 protons in a break-up volume of radius $R_{\text{break-up}} = 2.0 \times 141^{1/3}$ fm, as for the system $^{32}\text{S}+^{109}\text{Ag}$).

First, consider an evaluation of the ratio of densities of free neutron and free proton gases from the observed isobaric ratios $Y_{A,Z}/Y_{A,Z+1}$. Based on Eq. 8, one has

$$\frac{\rho_{nF}}{\rho_{pF}} = \frac{R_{\text{raw}}}{F_{\text{Coul}}}^{n/p}, \quad (9)$$

where $R_{\text{raw}}$ is the value of this ratio deduced in the absence of the Coulomb correction (i.e., given by the original ACCR [7] formalism) and $F_{\text{Coul}}^{n/p}$ is a correction factor resulting from the Coulomb term proposed in the present paper:

$$F_{\text{Coul}}^{n/p} = e^{\left[V_{pF}^{\text{coul}}(Z+1) - V_{pF}^{\text{coul}}(Z)\right]/T}, \quad (10)$$

Using Eqs. 10 and 7 and the values of $T=3.3$ MeV and $\rho_{pF} = 0.0011$ fm$^{-3}$, one obtains $F_{\text{Coul}}^{n/p} = 1.1$, for the case of the isobaric ratio $Y_{3,1}/Y_{3,2}$ (tritium - helium-3), $F_{\text{Coul}}^{n/p} = 1.28$, for the case of the isobaric ratio $Y_{13,6}/Y_{13,7}$, and $F_{\text{Coul}}^{n/p} = 1.59$ when the isobaric ratio $Y_{34,16}/Y_{34,17}$ is utilized. This example demonstrates that even in the favorable case of light isobars $^3\text{H}$ and $^3\text{He}$, the correction factor is large enough to mandate an inclusion of the proposed Coulomb correction term in the equation for the chemical equilibrium. Certainly, this correction factor is quite sizeable when yields of heavier isobars are utilized for the evaluation of the relative densities of free neutron and free proton gases.

It is worth noting that, according to Eq. 10, the Coulomb correction factor, $F_{\text{Coul}}^{n/p}$, for the relative densities of gases of free neutrons and protons is always greater than unity, since the exponent $[V_{pF}^{\text{coul}}(Z+1) - V_{pF}^{\text{coul}}(Z)]$ is positive. This fact reflects the role of the Coulomb energy in a neutron-enrichment of the free nucleon gas, a rather trivial effect that should not be confused with an isospin fractionation [8–10] driven by an isospin-dependent equation of state of nuclear matter.
As a second example, consider the evaluation of the break-up temperature \( T \) based on a double isotone ratio:

\[
R_{\text{isotone}} = \frac{Y_{A_1,Z_1}/Y_{A_1+1,Z_1+1}}{Y_{A_2,Z_2}/Y_{A_2+1,Z_2+1}}. \tag{11}
\]

In such a case, the breakup temperature \( T \) is ultimately evaluated from the experimentally determined value of the ratio

\[
\frac{\Delta B + \Delta V_{coul}^{pF}}{T} = \frac{\Delta B}{T_{\text{raw}}} = \ln(a R_{\text{isotone}}), \tag{12}
\]

where \( \Delta B = B_{A_1+1,Z_1+1} - B_{A_1,Z_1} + B_{A_2,Z_2} - B_{A_2+1,Z_2+1} \) and \( \Delta V_{coul}^{pF} = V_{coul}^{pF}(Z_1+1) - V_{coul}^{pF}(Z_1) + V_{coul}^{pF}(Z_2) - V_{coul}^{pF}(Z_2+1) \). The parameter \( a \) in Eq. (12) accounts for intrinsic partition functions \( \omega \) (see Eq. 5) of the isotones involved, and \( T_{\text{raw}} \) is the break-up temperature obtained using the original ACCR approach.

Eq. (12) allows one to express the relevant Coulomb correction factor \( F_{\text{Coul}}^T \) as

\[
F_{\text{Coul}}^T = \frac{T}{T_{\text{raw}}} = 1 + \frac{\Delta V_{coul}^{pF}}{\Delta B}. \tag{13}
\]

Using Eq. (13) the value of \( \rho_{pF} = .0011 \text{ fm}^{-3} \), and values of binding energies from the mass tables, one obtains \( F_{\text{Coul}}^T = 0.96 \) in the case when the experimental double isotone ratio \( (Y_{13,7}/Y_{12,6})/(Y_{4,2}/Y_{3,1}) \) is employed, \( F_{\text{Coul}}^T = 1.19 \) in the case of the isotone ratio \( (Y_{13,7}/Y_{12,6})/(Y_{10,5}/Y_{9,4}) \), and \( F_{\text{Coul}}^T = 0.31 \) in the case of the isotone ratio \( (Y_{14,8}/Y_{13,7})/(Y_{3,2}/Y_{2,1}) \). Again, the estimated magnitude of the Coulomb correction factor well warrants an inclusion of the Coulomb correction term in the ACCR formalism.

In summary, the importance of a Coulomb correction term to the equation for the chemical equilibrium between fragments and the gas of free nucleons has been demonstrated. The correction term restores the symmetry of the equation defining the equilibrium, when the mutual interaction energies of nucleons in both, bound and free states, are consistently accounted for as done with the more rigorous Eq. (4). While the proposed correction term has no effect on the determination of break-up temperatures based on double isotope ratios and may be small in some cases, its effects on the determination of break-up temperature from
isotone ratios and on the determination of the relative densities of free proton and neutron
gases may be quite substantial in some other cases. This correction is certainly important in
systematic studies of various experimental “thermometers” that, by design, include a large
variety of isotonic ratios.

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