Canonical treatment of particle production in HICs

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1 Average collision rates for strangeness-production processes

Used literature: [KKL+01, BMRS03, KMR86].

In relativistic heavy-ion collisions, when it comes to production of particles obeying an exact conservation law like the production of particles with strangeness, charm, or bottom, sometimes the treatment of the fireball-evolution kinetics with the grand-canonical ensemble is inapplicable, particularly if the produced particle numbers $\langle N_s \rangle \lesssim 1$, where we consider the production of strange particles, which always are produced in pairs with the same number of strange and an anti-strange quarks.

In the following we assume that the bulk medium can be described adequately by a fluid in local thermal equilibrium consisting of light particles. We describe the strangeness production with the Boltzmann equation

$$\begin{aligned} p^\mu \frac{\partial f_{s1}}{\partial x^\mu} = \frac{1}{(2\pi)^3} \frac{1}{g_s} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3 \vec{p}_2}{E_2} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3 \vec{p}_1'}{E_1'} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3 \vec{p}_2'}{E_2'} g_a g_b g_s g_{\bar{s}} [W_{s\bar{s} \leftarrow ab}(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}_1' \vec{p}_2') f_{a1}' f_{b2}' \\ - W_{ab \leftarrow s\bar{s}}(\vec{p}_1' \vec{p}_2' \leftarrow \vec{p}_1 \vec{p}_2) f_{s1} f_{\bar{s}2}]. \end{aligned} \tag{1}$$

Here, the notation $f_{s1} = f_s(t, \vec{x}, \vec{p}_1)$ is the phase-space distribution function for the particle carrying a strange quark, etc. Further for all four-momenta the on-shell condition like $p_1^0 = E_1 = \sqrt{m_1^2 + \vec{p}_1^2}$ is implied. The transition probability rates are defined by the invariant S"=matrix elements of the corresponding QFT description of the scattering process [Hee15],

$$W_{ab \leftarrow s\bar{s}}(p_1', p_2' \leftarrow p_1, p_2) = \frac{\left\langle |\mathscr{M}_{\text{loss}}(s,t)|^2 \right\rangle}{64\pi^2} \delta^{(4)}(p_1 + p_2 - p_1' - p_2'). \tag{2}$$

The average symbol around the squared matrix elements means that the "unpolarized matrix element" is averaged over spin and other intrinsic quantum numbers (like isospin, color in case of partonic degrees of freedom etc.) for both the final and initial states. In the following all degeneracy factors g_j are explicitly written. All quantities are understood to be evaluated in terms of the Mandelstam variables s and t with energy-momentum conservation and on-shell conditions implied.

The relation to the invariant scattering cross section for the reaction $s\bar{s} \rightarrow ab$ ("loss term") is thus as follows:

$$\begin{aligned} \mathrm{d}\sigma_{ab \leftarrow s\bar{s}} &= \frac{\mathrm{d}^3 \vec{p}_1'}{E_1'} \frac{\mathrm{d}^3 \vec{p}_2'}{E_2'} \frac{g_a g_b}{I} W(\vec{p}_1', \vec{p}_2' \leftarrow \vec{p}_1, \vec{p}_2) \\ &= \frac{\mathrm{d}^3 \vec{p}_1'}{E_1'} \frac{\mathrm{d}^3 \vec{p}_2'}{E_2'} \frac{g_a g_b}{I} \frac{\left\langle |\mathscr{M}_{\text{loss}}(s,t)|^2 \right\rangle}{64\pi^2} \delta^{(4)}(p_1 + p_2 - p_1' - p_2'). \end{aligned} \tag{3}$$

with the invariant flux

$$I=\sqrt{(\underline{p}_1\cdot\underline{p}_2)^2-m_1^2m_2^2}=\frac{1}{2}\sqrt{\lambda_{12}(s)}=p_{\text{cm}}\sqrt{s}, \tag{4}$$

$$\lambda_{12}(s)=[s-(m_1+m_2)^2][s-(m_1-m_2)^2]. \tag{5}$$

Since (3) is manifestly covariant, we can evaluate the integral over the energy-momentum conserving Dirac distribution in the center-momentum frame, $\vec{p}_1'=-\vec{p}_2'$, $E_1'+E_2'=\sqrt{s}$:

$$\mathrm{d}\sigma_{\text{loss}}=\frac{\mathrm{d}^3\vec{p}_1'}{E_1'E_2'}\frac{g_a g_b}{P_{\text{cm}}\sqrt{s}}\frac{\left\langle|\mathscr{M}_{\text{loss}}(s,t)|^2\right\rangle}{64\pi^2}\delta(E_1'+E_2'-\sqrt{s}). \tag{6}$$

Now from $E_1'^2=\vec{p}_1'^2+m_1^2$ we find $\mathrm{d}E_1'E_1'=d\,p_1'p_1$ and similarly for E_2'. Also we have $p_1'=p_2'=p_{\text{cm}}'$ and thus

$$\mathrm{d}(E_1'+E_2')=\mathrm{d}\sqrt{s}=\mathrm{d}p_{\text{cm}}'\frac{\sqrt{s}}{E_1'E_2'}. \tag{7}$$

Using this in (6) finally yields

$$\mathrm{d}\sigma_{\text{L}}=\mathrm{d}\Omega_1' g_a g_b\frac{p_{\text{cm}}'}{64\pi^2 s\,p_{\text{cm}}}\left\langle|\mathscr{M}_{\text{loss}}(s,t)|^2\right\rangle. \tag{8}$$

This result we can use for the integration over $\vec{p}_1'$ and $\vec{p}_2'$ in the loss-collision term for the particle number. We consider a single fluid element with macroscopically small proper volume V and take its rest frame as the computational frame for the following calculation. We assume that within this macroscopically small (but microscopically large) fluid element the medium is homogeneous and isotropic. Then we can multiply (1) by $g_s V/[(2\pi)^3E_1]$ and then integrate over $\vec{p}_1$ and the entire volume. The term $\vec{p}_1/E_1\cdot\vec{\nabla}$ vanishes by the use of Stokes's theorem due to the assumed isotropy and thus we get for the loss term

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}N_{s,\text{L}}=\frac{V g_s g_{\bar{s}} g_a g_b}{(2\pi)^6}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_1}{E_1}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_2}{E_2}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_1'}{E_1'}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_1}{E_1}\delta^{(4)}(\underline{p}_1+\underline{p}_2-\underline{p}_1'-\underline{p}_2')\\ \frac{\left\langle|\mathscr{M}_{\text{L}}|^2\right\rangle}{64\pi^2}f_{s1}f_{\bar{s}2}.\end{aligned} \tag{9}$$

Comparison with (3) shows that the integration over $\vec{p}_1'$ and $\vec{p}_2'$ is already done, we only have to take out the invariant-flux factor $I=\sqrt{s}\,p_{\text{cm}}=\sqrt{\lambda_{s\bar{s}}}/2$, and the remaining integral over $\mathrm{d}\Omega_1'$ yields the total cross section $\sigma_{\text{L}}(s)$, leading to

$$\frac{\mathrm{d}}{\mathrm{d}t}N_{s,\text{L}}=\frac{V g_s g_{\bar{s}}}{(2\pi)^6}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_1}{E_1}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_2}{E_2}\frac{\sqrt{\lambda_{s\bar{s}}}}{2}\sigma_{\text{L}}(s)f_{s1}f_{\bar{s}2}. \tag{10}$$

Now we assume that for integrating over this cross section we can assume that the s and $\bar{s}$ particles are in thermal equilibrium, describable by the grand-canonical ensemble with $\mu_s=0$, and use the so defined average thermal rate per s and $\bar{s}$ particles

$$\frac{L}{V}=\frac{V g_s g_{\bar{s}}}{(2\pi)^6\langle N_s\rangle_{\text{GC}}\langle N_{\bar{s}}\rangle_{\text{GC}}}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_1}{E_1}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}_2}{E_2}\frac{\sqrt{\lambda_{s\bar{s}}}}{2}\sigma_{\text{L}}(s)\exp[\beta(E_1+E_2)]. \tag{11}$$

We start with the evaluation of the grand-canonical average strange-particle numbers:

$$\langle N_s \rangle_{\mathrm{GC}} = g_s V \int_{\mathbb{R}^3} \frac{\mathrm{d}\vec{p}}{(2\pi)^3} \exp(-\beta E_p) = \frac{V}{2\pi^2} \frac{m_s^2}{\beta} \mathrm{K}_2(\beta m_s). \tag{12}$$

Here, K_2 is a modified Bessel function (see App. A).

To evaluate the integral in (11), we make the kinematical constraints, implicitly contained in the integrand, explicit by using appropriate δ distributions:

$$\begin{aligned} I &= \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_1}{E_1} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_2}{E_2} \frac{\sqrt{\lambda_{s\bar{s}}}}{2} \sigma_{\mathrm{L}}(s) \exp[\beta(E_1+E_2)] \\ &= \int_{\mathbb{R}^4} \mathrm{d}^4 \underline{p} \int_{s_{\mathrm{thr}}}^{\infty} \mathrm{d}x \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_1}{E_1} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_2}{E_2} \frac{\sqrt{\lambda_{s\bar{s}}}}{2} \sigma_{\mathrm{L}}(s) \exp[\beta P^0] \delta^{(4)}(\underline{P}-\underline{p}_1-\underline{p}_2)\delta(s-\underline{P}^2). \end{aligned} \tag{13}$$

Note that still the on-shell conditions $p_1^0 = E_1 = \sqrt{m_1^2+\vec{p}_1^2}$ and $p_2^0 = E_2 = \sqrt{m_2^2+\vec{p}_2^2}$ are tacitly assumed too.

Now we can make use of the manifest covariance of all these integrals and integrate out the δ distributions. We start with integrating out $\delta^{(4)}(\underline{P}-\underline{p}_1-\underline{p}_2)$. Since the integral is manifestly Lorentz invariant we can use the center-momentum frame, where $\vec{P}=0$ again and express everything in invariants. Making use of (7) for the unprimed momenta, we find

$$\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_1}{E_1} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}_2}{E_2} \delta^{(4)}(\underline{p}_1+\underline{p}_2-\underline{P}) = \frac{2\pi}{s}\sqrt{\lambda_{s\bar{s}}}. \tag{14}$$

Finally we need

$$\begin{aligned} \int_{\mathbb{R}^4} \mathrm{d}^4\underline{P} \exp(-\beta P^0)\delta(s-\underline{P}^2) &= 4\pi \int_{\sqrt{s}}^{\infty} \mathrm{d}P_0 \int_0^{\infty} \mathrm{d}P P^2 \delta(s-P_0^2 0-P^2) \\ &= 2\pi \int_{\sqrt{s}}^{\infty} \mathrm{d}P_0 \sqrt{P_0^2-s}\exp(-\beta P^0). \end{aligned} \tag{15}$$

By substitution of $P_0 = \sqrt{s}\cosh y$ we find

$$\begin{aligned} 2\pi \int_{\sqrt{s}}^{\infty} \mathrm{d}P_0 \sqrt{P_0^2-s}\exp(-\beta P^0) &= 2\pi s \int_0^{\infty} \mathrm{d}y \sinh^2 y \exp(-\beta\sqrt{s}\cosh y) \\ &= 2\pi s \int_0^{\infty} \mathrm{d}y (\cosh^2 y - 1)\exp(-\beta\sqrt{s}\cosh y) \\ &= \pi \int_0^{\infty} \mathrm{d}y [\cosh(2y)-1]\exp(-\beta\sqrt{s}\cosh y) \\ &= \pi s[\mathrm{K}_2(\beta\sqrt{s})-\mathrm{K}_0(\beta\sqrt{s})] = \frac{2\pi\sqrt{s}}{\beta}\mathrm{K}_1(\beta\sqrt{s}), \end{aligned} \tag{16}$$

where we have made use of (60) and (63). Using (12-16) in (11) we finally obtain

$$\begin{aligned} \frac{L}{V} &= \frac{\beta\int_{s_{\mathrm{thr}}}^{\infty} \mathrm{d}s \frac{1}{\sqrt{s}} \lambda_{s\bar{s}} K_1(\beta\sqrt{s})\sigma_L(s)}{8 m_s^2 m_{\bar{s}}^2 \mathrm{K}_2(\beta m_s)\mathrm{K}_2(\beta m_{\bar{s}})} \\ &= \frac{\beta\int_{\sqrt{s_{\mathrm{thr}}}}^{\infty} \mathrm{d}\sqrt{s}\, \lambda_{s\bar{s}} K_1(\beta\sqrt{s})\sigma_L(s)}{4 m_s^2 m_{\bar{s}}^2 \mathrm{K}_2(\beta m_s)\mathrm{K}_2(\beta m_{\bar{s}})}, \end{aligned} \tag{17}$$

where the threshold center-momentum energy is defined as

$$\sqrt{s_{\text{thr}}} = \max(m_A + m_B, m_s + m_{\bar{s}}). \tag{18}$$

Note that (17) deviates from the result given in [KMR86] by a factor of 2, which can be traced back to Eq. (5.10) in this paper, which should read (adapted to our notation)

$$v_{ab} 2E_s 2E_{\bar{s}} = 2\sqrt{\lambda_{s\bar{s}}}. \tag{19}$$

Our result is confirmed, e.g., in [BBLZ83, Can17]. In the same way one derives, taking into account the "detailed-balance identity" $\left\langle |\mathscr{M}_G|^2 \right\rangle = \left\langle |\mathscr{M}_L|^2 \right\rangle$,

$$G = \frac{g_s g_{\bar{s}} m_s^2 m_{\bar{s}}^2 \mathrm{K}_2(\beta m_s) \mathrm{K}_2(\beta m_{\bar{s}})}{g_A g_B m_A^2 m_B^2 \mathrm{K}_2(\beta m_A) \mathrm{K}_2(\beta m_B)} L. \tag{20}$$

2 Master equations

Now we consider the production of strange (charm, or bottom) particles in heavy-ion collisions. We assume that the "bulk matter" consisting of partons or hadrons in the light-(u,d)-quark sector are in local thermal equilibrium and the corresponding bulk medium is sufficiently well described by the local grand-canonical equilibrium ensemble, while the strange (charm, bottom) particles have to be described in each single event by the canonical ensemble, i.e., that there is a precise number $N_s = N_{\bar{s}}$ of particles containing strange and/or anti-strange quarks. The observables are an average of many such single events, and we ask for the time evolution of the corresponding average particle numbers, $\langle N \rangle = \langle N_s \rangle = \langle N_{\bar{s}} \rangle$. The most complete description is given by the Probabilities $P_n(t)$ to have precisely $n = N_s = N_{\bar{s}}$ particles in an event. The change of this probabilities is assumed to occur through $2 \leftrightarrow 2$ processes considered in the previous section with the gain and loss rates G/V and L/V, discussed above.

A gain process to have exactly n strange particles can be either the loss of an s-particle when before the reaction there have been $(n+1)$ s-particles (which occurs at the rate L/V) or a gain process having $(n-1)$ s-particles before the reaction (occuring at the rate G/V).

Analogously a loss process can either be having n s-particles before the collision and a loss process with rate L/V to $(n-1)$ s-particles or having n s-particles before the reaction leading to $(n+1)$ s-particles with a rate G/V.

For the "gain processes" $A + B \rightarrow s + \bar{s}$ we can use $\langle N_A \rangle_{\text{GC}}$ and $\langle N_B \rangle_{\text{GC}}$ as the particle numbers in the initial state, according to the assumption made above. The subscript GC stands for grand-canonical ensemble averages. We express then everything in terms of the loss rates,

$$G \langle N_A \rangle_{\text{GC}} \langle N_B \rangle_{\text{GC}} = \epsilon L. \tag{21}$$

Then the master equation reads

$$\begin{aligned} \dot{P}_n =& \frac{L}{V}(n+1)^2 P_{n+1} + \frac{\epsilon L}{V} P_{n-1} \quad (\text{"gain"}) \\ &- \frac{L}{V} n^2 P_n - \frac{\epsilon L}{V} P_n \quad (\text{"loss"}) \\ =& \frac{L}{V}\left[(n+1)^2 P_{n+1} - (n^2 - \epsilon) P_n + \epsilon P_{n-1}\right]. \end{aligned} \tag{22}$$

This is a system of first-oder differential equations of infinitely many functions, $P_n(\tau)$, where τ is the proper time since we evaluate everything in the rest frame of a fluid cell of proper volume V. The ODE system (22) can be transferred to a PDE for the generating function,

$$g(\tau,x)=\sum_{n=0}^{\infty} x^n P_n(\tau) \Leftrightarrow P_n(\tau)=\frac{1}{n!}\partial_x^n g(\tau,x)\Big|_{x=0}. \tag{23}$$

Multiplying the master equation (22) with x^n and summing over all n (where of course by definition on the left-hand side $P_{-1}(\tau)\equiv 0$) one finds the PDE

$$\partial_\tau g=\frac{L}{V}(1-x)(x\partial_x^2 g+\partial_x g-\epsilon g). \tag{24}$$

Note that for $x=1$ we get $\partial_\tau g(\tau,1)=0$, as it must be since $g(\tau,1)=\sum_n P_n(\tau)=1=\text{const.}$ To gain complete statistical information of the stochastic process of strange-particle production one has to solve (24) with a given initial function $g(0,x)=g_0(x)$, equivalent to the probabilities $P_n(0)$ at $\tau=0$.

Unfortunately there is no simple general solution for (24). Nevertheless we can solve for the equilibrium solution, which is reached in the long-time limit $\tau\rightarrow\infty$. It is given by $\partial_\tau g_{\text{eq}}=0$. With (24) we get ODE

$$x\,g_{\text{eq}}''(x)+g_{\text{eq}}'(x)-\epsilon\, g_{\text{eq}}=0. \tag{25}$$

Using the new independent variable $y=2\sqrt{\epsilon x}$ and $g_{\text{eq}}(x)=G[y(x)]=G[2\sqrt{\epsilon x}]$ (25) transforms into the modified Bessel differential equation (58) with $m=0$:

$$y^2G''(y)+yG'(y)-y^2G(y)=0. \tag{26}$$

Since $G(0)=g_{\text{eq}}(0)=P_0^{(\text{eq})}$ is finite, the unique solution is

$$g_{\text{eq}}(x)=\frac{\mathrm{I}_0(2\sqrt{\epsilon x})}{\mathrm{I}_0(2\sqrt{\epsilon})}, \tag{27}$$

where we have used the normalization condition $g_{\text{eq}}(1)=1$ to determine the overall factor.

By expanding the exponential function in the defining equation (59) and working out the integrals one finds the series expansion,

$$\mathrm{I}_m(x)=\sum_{j=0}^{\infty}\frac{1}{j!(j+m)!}\left(\frac{x}{2}\right)^{2j+m}, \tag{28}$$

and particularly for $m=0$

$$\mathrm{I}_0(2\sqrt{\epsilon x})=\sum_{j=0}^{\infty}\frac{\epsilon^j}{(j!)^2}x^j. \tag{29}$$

From this one reads off

$$P_n^{(\text{eq})}=\frac{\epsilon^n}{(n!)^2\mathrm{I}_0(2\sqrt{\epsilon})}. \tag{30}$$

The expectation value of produced strange-antistrange particle pairs averaged over many collisions is easily calculated since

$$\langle N_s\rangle_{\text{eq}}^{(\text{can})}=g_{\text{eq}}'(1)=\sqrt{\epsilon}\frac{\mathrm{I}_1(2\sqrt{\epsilon})}{\mathrm{I}_0(2\sqrt{\epsilon})}, \tag{31}$$

where we have used (63 for $m = 0$.

We note that with (24) we can easily derive the rate equation for the mean strange-particle number by using

$$\partial_x g(\tau, x)|_{x=1} = \sum_{n=0}^{\infty} n x^{n-1} P_n(\tau)\Big|_{x=1} = \langle n \rangle, \tag{32}$$

$$\partial_x^2 g(\tau, x)|_{x=1} = \sum_{n=0}^{\infty} n(n-1) x^{n-2} P_n(\tau)\Big|_{x=1} = \langle n(n-1) \rangle. \tag{33}$$

Thus, applying ∂_x on Eq. (24) and setting $x = 1$ we find the rate equation

$$\mathrm{d}_\tau \langle N_s \rangle_{\text{can}} = -\frac{L}{V} \left(\langle N_s^2 \rangle_{\text{can}} - \epsilon \right). \tag{34}$$

Note that this is not a closed equation for $\langle N_s \rangle$, because on the right-hand side we have $\left\langle N_s^2 \right\rangle$ which can, in this exact canonical treatment, not expressed in terms of $\langle N_s \rangle$. The only conclusion we can draw is that in the equilibrium limit, where the left-hand side of (34) vanishes,

$$\left\langle N_s^2 \right\rangle_{\text{can}}^{(\text{eq})} = \epsilon. \tag{35}$$

3 Grand-canonical approximation

Treating also the $\bar{s}$ particles in the grand-canonical approximation when deriving the master equation for the probabilities P_n, leads to simpler relations, but one should note that this approximation is only valid if $\langle N_s \rangle_{\text{GC}} = \langle N_s \rangle_{\text{GC}} \gg 1$. In this derivation for the single event we assume that the $\bar{s}$-particle number can be approximated by $\langle N_{\bar{s}} \rangle_{\text{GC}}$. The s"=particle number can fluctuate since in the grand-canonical ensemble strangeness conservation is fulfilled only on the average.

We have to start from the same arguments leading to (22), but wherever the $\bar{s}$-particle number enters we have to use $\langle N_{\bar{s}} \rangle_{\text{GC}} = \langle N_s \rangle_{\text{GC}}$ leading to the master equation,

$$\mathrm{d}_\tau P_n = \frac{L}{V} \left[\langle N_s \rangle_{\text{GC}} (n+1) P_{n+1} - \left(\langle N_s \rangle_{\text{GC}}\, n + \epsilon \right) P_n + \epsilon P_{n-1} \right]. \tag{36}$$

Multiplying by x^n and summing over n leads to the master equation for the generating function,

$$\partial_\tau g_{\text{GC}}(\tau, x) = \frac{L}{V}(1-x) \left(\langle N_s \rangle_{\text{GC}}\, \partial_x g_{\text{GC}} - \epsilon\, g_{\text{GC}} \right). \tag{37}$$

Taking the derivative wrt. x and then setting $x = 1$ leads to the rate equation

$$\mathrm{d}_\tau \langle N \rangle = -\frac{L}{V} \left(\langle N \rangle_{\text{GC}} \langle N \rangle - \epsilon \right). \tag{38}$$

In equilibrium we find

$$\langle N \rangle_{\text{eq}} = \langle N_s \rangle_{\text{GC}} = \sqrt{\epsilon}. \tag{39}$$

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[1]This is in accordance with (31) since for $\epsilon \to \infty$ the Bessel functions behave asymptotically as

$$\mathrm{I}_m(x) \underset{x \to \infty}{\cong} \frac{\exp x}{\sqrt{2\pi x}},$$

independent of n.

Thus we can write (37) in the form

$$\partial_\tau g_{\text{GC}} = \frac{L}{V}\sqrt{\epsilon}(1-x)(\partial_x g_{\text{GC}} - \sqrt{\epsilon}\, g_{\text{GC}}). \tag{40}$$

The equilibrium limit thus is

$$g_{\text{GC}}^{(\text{eq})}(x) = \exp[\sqrt{\epsilon}(x-1)]. \tag{41}$$

The probabilities are

$$P_n = \frac{1}{n!}\partial_x^n g_{\text{GC}}^{(\text{eq})} = \frac{\exp(-\sqrt{\epsilon})}{n!}\sqrt{\epsilon}^n, \tag{42}$$

i.e., the expected Poisson distribution for the s-particle number in the grand-canonical ensemble with an average of $\sqrt{\epsilon}$.

Since (40) is a 1st-order PDE it is easily solved by the method of characteristics. We like to solve the equation for an arbitrary initial condition,

$$g_{\text{GC}}(0,x) = g_0(x). \tag{43}$$

To that end we make $\tau = \tau(\lambda)$, $x = x(\lambda)$, $g = g[\tau(\lambda), x(\lambda)]$ with a parameter λ. This gives

$$\mathrm{d}_\lambda g_{\text{GC}} = (\mathrm{d}_\lambda \tau)\partial_\tau g + (\mathrm{d}_\lambda x)\partial_x g. \tag{44}$$

Comparing with (40) we find the set of ODEs for the characteristics of the master equation (40) (with $\gamma = L/V$)

$$\mathrm{d}_\lambda \tau = 1, \quad \mathrm{d}_\lambda x = -\sqrt{\epsilon}\gamma(1-x), \quad \mathrm{d}_\lambda g_{\text{GC}} = \epsilon\gamma(1-x). \tag{45}$$

This set we solve, imposing the initial conditions,

$$\tau(0) = 0, \quad x(0) = x_0, \quad g_{\text{GC}}(0, x_0) = g_0(x_0), \tag{46}$$

to

$$\tau = \lambda, \quad x = 1 + (x_0 - 1)\exp(\gamma\sqrt{\epsilon}\lambda), \quad g_{\text{GC}} = g_0(x_0)\exp\left\{\sqrt{\epsilon}(1-x_0)\left[\exp(\lambda\sqrt{\epsilon}\lambda - 1)\right]\right\}. \tag{47}$$

The inverse transformation $(\lambda, x_0) \rightarrow (\tau, x)$ finally gives the solution

$$g_{\text{GC}}(\tau, x) = g_0\left[1 + (x-1)\exp(-\gamma\sqrt{\epsilon}\tau)\right]\exp\left\{\sqrt{\epsilon}(x-1)\left[1 - \exp(-\gamma\sqrt{\epsilon}\tau)\right]\right\}. \tag{48}$$

The relaxation time in this case obviously is

$$\tau_{\text{rel}} = \frac{1}{\gamma\sqrt{\epsilon}}. \tag{49}$$

Note that for $\tau \rightarrow \infty$, we indeed get the equilibrium result (41). The rate equation (38), using (39) has the solution

$$\langle N \rangle = \sqrt{\epsilon} + (\langle N_0 \rangle - \sqrt{\epsilon})\exp(-\gamma\sqrt{\epsilon}\tau). \tag{50}$$

4 Ultracanonical limit

Another limit, leading to an analytically solvable master equation, is the "ultra-canonical limit", i.e., when $\langle N_s \rangle_{\text{GC}} \ll 1$. Then we have $P_n \ll P_0, P_1$ for $n \geq 2$ at all times, and thus we can neglect $x \partial_x^2 g$ in (24),

$$\partial_\tau g_{\text{UC}} = \gamma(1-x)(\partial_x g_{\text{UC}} - \epsilon g_{\text{UC}}), \quad \gamma = \frac{L}{V}, \tag{51}$$

which is of the same form as (37). The method of characteristics gives the solution of the general initial-value problem.

$$g_{\text{UC}}(\tau, x) = g_0 [1 + (x-1)\exp(-\gamma\tau)] \exp\{\epsilon(x-1)[1-\exp(-\gamma\tau)]\}. \tag{52}$$

Obviously the relaxation time in this case is $\tau_{\text{rel}} = 1/\gamma$.
The rate equation reads

$$\mathrm{d}_\tau \langle N \rangle_{\text{UC}} = -\gamma(\langle N \rangle_{\text{UC}} - \epsilon) \tag{53}$$

with the solution

$$\langle N \rangle_{\text{UC}} = \epsilon + (\langle N_0 \rangle - \epsilon) \exp(-\gamma\tau) \tag{54}$$

with the equilibrium limit[2]

$$\langle N \rangle_{\text{UC}}^{(\text{eq})} = \epsilon. \tag{55}$$

5 Remark on the "standard GC rate equation"

In the literature (e.g., [KKL$^+$01, BMRS03]) one finds a rate equation for $\langle N_s \rangle_{\text{GC}} \gg 1$, using the "approximation" $\langle N^2 \rangle \simeq \langle N \rangle^2$ in (34):

$$\mathrm{d}_\tau \langle N \rangle = -\gamma(\langle N \rangle^2 - \epsilon). \tag{56}$$

This is plausible since at least close to equilibrium one can assume that $\Delta N^2 = \langle N^2 \rangle - \langle N \rangle^2 \simeq \langle N \rangle$ as for the Poisson distribution valid in the grand-canonical equilibrium limit. If $\langle N \rangle \gg 1$ this justifies the approximation $\langle N^2 \rangle = \langle N \rangle^2 + \langle N \rangle \simeq \langle N \rangle^2$. Its general solution reads

$$\langle N \rangle = \sqrt{\epsilon} \tanh\left[\sqrt{\epsilon}\gamma\tau + \operatorname{artanh}\left(\frac{\langle N_0 \rangle}{\sqrt{\epsilon}}\right)\right]. \tag{57}$$

From this one also reads off the typical relaxation-time scale (49) and the equilibrium limit $\langle N \rangle^{(\text{eq})} = \sqrt{\epsilon}$ in accordance with (49) and (39), respectively.

[2]This is in accordance with (31) since for $\sqrt{\epsilon} \ll 1$ we can use the asymptotics of the Bessel functions,

$$\mathrm{I}_n(x) \underset{x \to 0}{\cong} \frac{1}{m!}\left(\frac{x}{2}\right)^m$$

A Modified Bessel functions

In this Appendix we quickly summarize the properties of the modified Bessel functions [OLBC10, CH10]. We define them as two linearly independent solutions of the modified Bessel equation,

$$x^2 y''(x) + x y'(x) - (x^2 + m^2) y(x) = 0. \tag{58}$$

For our applications the following integral representations are particularly useful. We restrict ourselves to $m \in \mathbb{N}_0$:

$$\mathrm{I}_m(x) = \frac{1}{\pi} \int_0^{\pi} \mathrm{d}\varphi \cos(mx) \exp(x \cos\varphi) \tag{59}$$

$$\mathrm{K}_m(x) = \int_0^{\infty} \mathrm{d}y \cosh(my) \exp(-x \cosh y). \tag{60}$$

For $m \geq 0$ the function $\mathrm{I}_m(x)$ is regular in $x = 0$ and exponentially increasing for $x \to \infty$, while K_m is singular at $x = 0$ and exponentially decreasing for $x \to \infty$.
They fulfill the following relations,

$$\mathrm{I}_{m+1}(x) - \mathrm{I}_{m-1}(x) = -\frac{2m}{x} \mathrm{I}_m(x), \tag{61}$$

$$\mathrm{K}_{m+1}(x) - \mathrm{K}_{m-1}(x) = \frac{2m}{x} \mathrm{K}_m(x). \tag{62}$$

The derivatives are

$$\mathrm{I}'_m(x) = \frac{1}{2}[\mathrm{I}_{m+1}(x) + \mathrm{I}_{m-1}(x)] = \mathrm{I}_{m+1}(x) + \frac{m}{x} \mathrm{I}_m(x), \tag{63}$$

$$\mathrm{K}'_m(x) = -\frac{1}{2}[\mathrm{K}_{m+1}(x) + \mathrm{K}_{m-1}(x)] = -\mathrm{K}_{m+1}(x) - \frac{m}{x} \mathrm{K}_m(x). \tag{64}$$

Both can be derived easily from the definitions (59) and (60).

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