A kinetic equation which combines the quasiparticle drift of Landau’s equation with a dissipation governed by a nonlocal and noninstantaneous scattering integral in the spirit of Enskog corrections is discussed. Numerical values of the off-shell contribution to the Wigner distribution, of the collision duration and of the collision nonlocality are presented for different realistic potentials. On preliminary results we show that simulations of quantum molecular dynamics extended by the nonlocal treatment of collisions leads to a broader proton distribution bringing the theoretical spectra closer towards the experimental values than the local approach.

1 Introduction

One of the long standing problems in nuclear physics is to find the equation of state of nuclear matter [1]. In the absence of any direct measurement, it is hoped that the equation of state can be deduced from heavy ion reactions via dynamical simulation of the fragmentation scenario. Most simulations rely on the local and instantaneous treatment of binary collisions as they appear in the Boltzmann equation

\[ \frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k} \frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r} \frac{\partial f_1}{\partial k} = \sum_b \int \frac{dp dq}{(2\pi)^5} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) |T_{ab}(\varepsilon_1 + \varepsilon_2, k, p, q, t, r)|^2 \times \left[f_3 f_4 (1-f_1)(1-f_2) - (1-f_3)(1-f_4)f_1 f_2 \right]. \]  

The arguments of distributions \( f \) and energies \( \varepsilon \) are shortened as \( f_1 \equiv f_a(k, r, t), f_2 \equiv f_b(p, r, t), f_3 \equiv f_a(k - q, r, t), \) and \( f_4 \equiv f_b(p + q, r, t), \) with momenta \( k, p, q, \) coordinate \( r, \) time \( t, \) and spin and isospin \( a, b. \) The local picture of the collision is reflected by the same coordinate \( r \) at all distributions, the instantaneous by the same time \( t. \)

A real binary collision is neither local nor instantaneous. A nonlocal picture of a collision is schematically drawn in figure [4]. Let us introduce individual nonlocal corrections step by step for simple but useful models. The first nonlocal corrections have been introduced by Enskog for the classical gas of hard spheres [2]. The collision of hard spheres is instantaneous so that each trajectory is broken only at a single point. Accordingly, in figure [4] \( \Delta_3 = 0 \) and \( \Delta_4 - \Delta_2 = 0, \) i.e., \( \Delta_t = 0 \) and \( \Delta_\phi = 0. \) At the instant of the collision, the particles are displaced by the sum of their radii in the
direction of the transferred momentum what is described by a nonzero vector $\Delta_{HS}$. Corresponding changes in the kinetic equation enter the position of the ongoing particle, $f_2 = f_b(p, r - \Delta_{HS}, t)$ and $f_4 = f_b(p + q, r - \Delta_{HS}, t)$ while other arguments remain unchanged. The equation of state evaluated from the kinetic equation with the nonlocal scattering integral is of the van der Waals type covering the excluded volume [2, 3]. For nuclear matter, Enskog’s corrections have been first discussed by Malfliet [4] and recently implemented by Kortemayer, Daffin and Bauer [5].

Another simple model one obtains assuming that colliding particles form an unstable molecule of an average time of life $\Delta_t$ called the collision duration or the collision delay. Neglecting the size of the molecule, $\Delta_2 = 0$ and $\Delta_4 - \Delta_3 = 0$, i.e., $\Delta_{HS} = 0$ and $\Delta_\phi = 0$, the only nonzero displacement $\Delta_t$ measures a distance between points where molecule forms and breaks up. This distance is given by $\Delta_t = \Delta_t v^{\text{mol}}$ with the molecular velocity $v^{\text{mol}} = (k + p)/(m_a + m_b)$. Corresponding changes in the kinetic equation enter the time argument and positions of final states, $f_3 = f_a(k - q, r - \Delta_t, t - \Delta_t)$ and $f_4 = f_b(p + q, r - \Delta_t, t - \Delta_t)$. In the equation of state, the collision duration results in the same kind of terms as the presence of stable molecules. The finite duration of nucleon-nucleon collisions and its thermodynamic consequences has been studied by Schmidt, Röpke and Schulz [6], its effect on the pressure has been discussed only recently by Danielewicz and Pratt [7]. The noninstantaneous scattering integral and its consequences for the linear response has been first discussed for electrons in semiconductors scattered by resonant levels [8].

In a real collision, the two particles keep a finite distance, $\Delta_{HS} \neq 0$, and interact for a finite time, $\Delta_t \neq 0$ and $\Delta_t \neq 0$. Moreover, particles rotate one against the other as described by the rotation displacement $\Delta_\phi$. Consequently we obtain the following scenario of Fig. 1: Two particles approach until they reach a distance $\Delta_2$. Then they form a molecule living for $\Delta_t$ and traveling over a distance $\Delta_f$. During this propagation the molecule rotate as given by $\Delta_\phi$. Collecting all three shifts we obtain the nonlocal and noninstantaneous kinetic equation (6) derived in [8] with the help of the method introduced in [8]. The resulting arguments of the kinetic equation read finally $f_1 = f_a(k, r, t)$,
While the above microscopic picture of nonlocal and noninstantaneous isolated collisions is intuitively clear, it is less transparent how to define the same corrections for quasiparticles which carry a part of the interaction in the quasiparticle reconstruction of their energies and wave function norms. This question requires a systematic approach as it was first presented in [9]. This derivation follows Baerwinkel [11] in starting from nonequilibrium Green’s functions and keeping all gradient contributions to the scattering integral, but instead of the quasiparticle approximation, the extended quasiparticle approximation is used. Here we use numerical results to discuss the key steps and consequences of this approach.

2 Kinetic equation

We start our derivation of the kinetic equation from the quantum transport equation for the nonequilibrium Green’s functions first obtained by Kadanoff and Baym, see [12],

\[ -i \left[ G_0^{-1} - \text{Re}\Sigma, G^< \right] - i \left[ \text{Re}G, \Sigma^< \right] = \frac{1}{2} \{ G^>, \Sigma^< \} - \frac{1}{2} \{ G^<, \Sigma^> \}, \]

(2)

where \([,]\) and \(\{,\}\) denote commutators and anticommutators, \(\text{Re}G = \frac{1}{2}(G^R + G^A)\) is the hermitian part of the propagator. The center of interest is the particle correlation function \(G^<(1, 2) = \text{Tr} \left( \hat{\rho} \Psi^\dagger(2) \Psi(1) \right)\). Its time evolution, however, requires to know the accessible states given by the hole correlation function \(G^>(1, 2) = \text{Tr} \left( \hat{\rho} \Psi(1) \Psi^\dagger(2) \right)\), and a dynamics of interactions specified by the selfenergy \(\Sigma\). Individual terms in (2) have specific physical content. The \(G_0^{-1}\) describes a free motion of particles and is renormalized by \(\text{Re}\Sigma\). The \(\text{Re}G\) describes the off-shell motion after the collision. The first and second anticommutators are the scattering-in and -out.

The dynamics of interaction reflects selected models and approximations. For simplicity we assume that protons and neutrons are of equal mass \(m\), interact via an instant potential \(V\), and there is no spin-flipping mechanism. As common, the self-energy is constructed from retarded and advanced two-particle T-matrices \(T^{R, A}\) in the Bethe-Goldstone approximation [12] as

\[ \Sigma^<(1, 2) = T^R(13, 56)T^A(78, 24)G^>(4, 3)G^<(5, 7)G^<(6, 8), \]

(3)

and \(\Sigma^>\) is obtained from (3) by an interchange \(\leftrightarrow\). Numbers are cumulative variables, \(1 \equiv (t_1, r_1, a_1)\), and bars denote internal variables that are integrated over. Missing commas in arguments signal that the time arguments are identical, e.g., \(t_3 = t_1\) and \(t_5 = t_6\), the T-matrices are thus double-time functions. The approximations of set (3) are specified in the mixed representation, [off-diagonal elements in spin and isospin are excluded, \(a_1 = a_2 = a\)]

\[ G^<(1, 2) = \int \frac{d\omega}{2\pi} \frac{dk}{(2\pi)^3} e^{ik(r_1-r_2)-i\omega(t_1-t_2)} G^<_a (\omega, k, r, t) \]
2.1 Off-shell motion

Equations (2-3) completed with the Dyson equation for $G^R$ and the ladder equation for $T^R$ form a closed set for $G^<$. This set is converted to equations for the quasiparticle distribution $f$ with the help of the extended quasiparticle approximation [14, 13, 15, 16]

$$G^{<}_{1,\omega} = \left(1 - \frac{f_1}{f_1}\right)2\pi z_1 \delta(\omega - \varepsilon_1) + \text{Re} \frac{\Sigma^{<}_{1,\omega}}{(\omega - \varepsilon_1)^2},$$  \hspace{1cm} (5)

where $G_{1,\omega} \equiv G_a(\omega, k, r, t)$ and similarly $\Sigma$. The first term is singular and provides the dominant quasiparticle contribution on the energy shell. The second term is regular and contributes out of the energy shell. The approximative form of this off-shell contribution is consistent with the lowest approximation of the wave-function renormalization, $z_1 = 1 + \frac{\partial}{\partial \omega} \text{Re} \Sigma_1 |_{\varepsilon_1}$. Before we employ the extended quasiparticle approximation (5) to convert the transport equation (2) into a kinetic equation, it is useful demonstrate its physical content. The amplitude of the off-shell contributions and the need to treat them separately as in (5) can be seen in figure 2 where we compare the Wigner distribution $\rho_1 = \frac{1}{2\pi} \int d\omega G^{<}_{1,\omega}$ obtained from the exact equilibrium correlation functions $G^{<}$ with its extended quasiparticle approximation (5) and the plain quasiparticle approximation $G^{<}_{1,\omega} = f_1 2\pi \delta(\omega - \varepsilon_1)$ which yields the Fermi-Dirac distribution. We note that the simple Yamaguchi potential [17] has been used in the T-matrix for this comparison. One can see that the off-shell contribution given by the difference between the Wigner and the Fermi-Dirac distributions is not small, in particular at the high momenta region where the power-law off-shell tails always dominate over the exponentially falling quasiparticle distribution. Formula (5) provides inevitable and sufficiently precise off-shell corrections.

Out of equilibrium one has to evaluate $\Sigma^<$ which is similar to an evaluation of the scattering integral. From the extended quasiparticle approximation one then obtains the high-momenta tails found by Danielewicz [18] and Köhler [19] in direct numerical treatments of non-equilibrium Green’s functions.

Figure 2: The equilibrium occupation of momentum states given by Wigner’s distribution $\rho$ (full line) is compared with the quasiparticle distribution $f$ (long dashed line) and with the extended quasiparticle approximation (short dashed line) at the temperature $T = 10$ MeV.
2.2 Quasiclassical trajectories

Now we substitute (4) into (2) and neglect all gradient terms but linear. Within nuclear physics, the gradient expansion of the self-energy (3) is commonly omitted since it is a tedious task. It results in one nongradient and nineteen gradient terms that are analogous to those found within the chemical physics [20, 21]. All these terms can be recollected into a nonlocal and noninstantaneous scattering integral that has an intuitively appealing structure of a nonlocal Boltzmann equation (1)

$$\frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k} \frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r} \frac{\partial f_1}{\partial k} = \sum_b \int \frac{dp dq}{(2\pi)^5} \delta (\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4 + 2\Delta_E) \left(1 - \frac{1}{2} \frac{\partial \Delta_2}{\partial r} - \frac{\partial \varepsilon_2}{\partial r} \frac{\partial \Delta_2}{\partial \omega} \right)$$

$$\times \ z_1 z_2 z_3 z_4 |T_{ab}(\varepsilon_1 + \varepsilon_2 - \Delta_E, k - \frac{\Delta_K}{2}, p - \frac{\Delta_K}{2}, q, r - \Delta_r, t - \Delta_t)|^2$$

$$\times \ [f_4 f_4 (1 - f_1)(1 - f_2) - (1 - f_3)(1 - f_4)f_1 f_2].$$  (6)

with Enskog-type shifts of arguments [1, 10]: $f_1 \equiv f_a(k, r, t)$, $f_2 \equiv f_b(p, r - \Delta_2, t)$, $f_3 \equiv f_a(k - q - \Delta_K, r - \Delta_3, t - \Delta_t)$, and $f_4 \equiv f_b(p + q - \Delta_K, r - \Delta_4, t - \Delta_t)$. In agreement with [20, 21], all gradient corrections result proportional to derivatives of the scattering phase shift $\phi = \text{Im} \ln T_{ab}(\Omega, k, p, q, t, r)$,

$$\Delta_2 = \left(\frac{\partial \phi}{\partial p} - \frac{\partial \phi}{\partial q} - \frac{\partial \phi}{\partial k}\right)_{\varepsilon_1 + \varepsilon_4} \Delta_3 = -\left(\frac{\partial \phi}{\partial k}\right)_{\varepsilon_1 + \varepsilon_4} \Delta_4 = -\left(\frac{\partial \phi}{\partial k} + \frac{\partial \phi}{\partial q}\right)_{\varepsilon_3 + \varepsilon_4}$$

$$\Delta_t = \left(\frac{\partial \phi}{\partial t}\right)_{\varepsilon_3 + \varepsilon_4} \Delta_E = -\frac{1}{2} \left(\frac{\partial \phi}{\partial t}\right)_{\varepsilon_3 + \varepsilon_4} \Delta_K = \frac{1}{2} \left(\frac{\partial \phi}{\partial r}\right)_{\varepsilon_3 + \varepsilon_4},$$  (7)

and $\Delta_r = \frac{1}{4}(\Delta_2 + \Delta_3 + \Delta_4)$. After derivatives, $\Delta$’s are evaluated at the energy shell $\Omega \rightarrow \varepsilon_3 + \varepsilon_4$.

For the purpose of discussion, it is advantageous to link the quantum displacements (7) to intuitively more appealing hard-sphere and rotation shifts by relations obvious from figure [1]

$$\Delta_{HS} = \frac{1}{2}(\Delta_4 - \Delta_3 + \Delta_2), \quad \Delta_\phi = \frac{1}{2}(\Delta_4 - \Delta_3 - \Delta_2).$$  (8)

For the collision of two isolated nucleons, it is possible to show that $\Delta_{HS}$ points in the direction of the transferred momentum $q$. Similarly it follows that the rotation shift is orthogonal to $\Delta_{HS}$ and stays in the collision plane.

In figure [3] we plot the delay time and the amplitude of the hard-sphere shift for different deflection angles versus lab energy. The T-matrix is evaluated with different potentials, Bonn (A-C) [22], Paris [23] and separable Paris [24], concerning partial wave coupling up to D-waves [25]. The forward angle delay time has a negative minimum at small energies indicating an attractive behavior. For very small energies the delay time is rapidly decreasing to high negative values reflecting the occurrence of weakly bound states. The sharp jump for $\theta = 90^\circ$ is caused by a resonant character of this scattering channel. Its value is misplaced and exaggerated within the separable approximation. The hard core shift $\Delta_{HS}$ behaves regularly at low energies. The resonant scattering at $\theta = 90^\circ$ appears as the increase of the amplitude. Again, the separable potential exaggerates its value. Characteristic values $\Delta_t \sim 1 \text{ fm/c}$
3 Implementation in heavy ion codes

The selfconsistent evaluation of all $\Delta$’s would be as demanding as the full Green’s function treatment of the system. We employ two kinds of additional approximations. First, following the approximations used within the Boltzmann equation, we neglect the medium effect on binary collision, i.e., use the well known free-space T-matrix. Second, we rearrange the scattering integral into an instantaneous but nonlocal form. To eliminate the time delay from distributions we neglect collisions on the time scale $\Delta_t$ and shift arguments of distributions along the trajectory of a particle. In the differential form this step derives as

$$f_a(k - q - \Delta_k, r - \Delta^3_r, t - \Delta_t) = f_a(k - q - \Delta_k, r - \Delta^3_r, t) - \frac{\partial f_3}{\partial t} \Delta_t$$

$$= f_a(k - q - \Delta_k - \frac{\partial \varepsilon_3}{\partial k} \Delta_t, r - \Delta_3 + \frac{\partial \varepsilon_3}{\partial k} \Delta_t, t). \quad (9)$$

In the last step we have used the collision-free kinetic equation $\frac{\partial f_3}{\partial t} + \frac{\partial \varepsilon_3}{\partial k} \frac{\partial f_3}{\partial r} - \frac{\partial \varepsilon_3}{\partial r} \frac{\partial f_3}{\partial k} = 0$. With approximation (9) and similar for $f_4$, the scattering integral (8) corresponds to an instantaneous event at time $t$. The collision remains nonlocal with modified space displacements of particles at initial states

$$\tilde{\Delta}_{3,4} = \Delta_{3,4} - \frac{\partial \varepsilon_{3,4}}{\partial k} \Delta_t. \quad (10)$$
The instantaneous approximation brings further simplifications following from conservation laws. During the instantaneous process, mean fields have no time to pass any momentum and energy to the colliding pair. Indeed, assuming the effect on colliding particles only via mean fields, from (7) one finds 
\[ \Delta_k = -\frac{\partial \epsilon_3,4}{\partial r} \Delta_t \] so that the momentum gain vanishes in (9). Similarly, the energy gain \( \Delta_E \) vanishes when arguments of quasiparticle energies in the energy conserving \( \delta \) function are brought to the same time instant. Finally, in agreement with the continuity of the center of mass motion, one finds that 
\[ \Delta_2 = \tilde{\Delta}_3 + \tilde{\Delta}_4. \] The scattering-in thus simplifies as 
\[ \sum_b \int \frac{dp}{(2\pi)^3} \frac{dq}{(2\pi)^3} 2\pi \delta (\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) |T_{ab}|^2 (k - p, q) f_3 f_4 (1 - f_1)(1 - f_2), \] (11)
where new arguments of energies and distributions are shifted only in space, 
\[ f_1 = f_a(k, r, t), \quad f_2 = f_b(p, r - \Delta_2, r, t), \quad f_3 = f_a(k - q, r - \tilde{\Delta}_3, t) \] and 
\[ f_4 = f_b(p + q, r - \tilde{\Delta}_4, t). \] The scattering-out is similar. In the T-matrix we have reduced arguments to those which are relevant for free-space collisions. Finally, we would like to stress that the amplitudes of displacements are not fitting parameters or a matter of an educated guess but evaluated from the T-matrix, i.e., from an interaction potential.

In order to investigate the effect of nonlocal collisions in realistic situations, we have evaluated \( \Delta \)'s from the separable Paris potential \[24\] and implemented the nonlocal scattering integral of (11) in a QMD code for the central collision of \( ^{129}\text{Xe}\rightarrow^{119}\text{Sn} \) at 50 MeV/A with and without non-local corrections. Figure 4 shows the exclusive proton spectra subtracting the protons bound in clusters. This procedure is performed within a spanning tree model which is known to describe a production of light charged cluster in a reasonable agreement with the experimental data. Within the local approximation, however, the remaining distribution of high-energy protons is too low to meet the experimental values. As one can see, the inclusion of nonlocal
collisions corrects this shortage of the QMD simulation. The increase in the high-energy part follows from an enhancement of a number of collisions at the pre-equilibrium stage of the reaction while later stages are not strongly affected [20]. Accordingly, the production of light clusters is rather insensitive to the nonlocal corrections. The improvement of the proton production is thus not on cost of worse results in other spectra.

4 Thermodynamic properties

The production of high-energy particles documents a vital role of nonlocal treatment far from equilibrium. Their role can be best seen on thermodynamic observables like density $n_a$ of particles $a$, density of energy $E$, and the stress tensor $J_{ij}$ which conserve within the nonlocal and noninstantaneous kinetic equation (9). Integrating (9) over momentum $k$ with factors $\varepsilon_1$, $k$ and unity one finds [9, 10] that each observable has the standard quasiparticle part following from the drift

$$E_{\text{qp}} = \sum_a \int \frac{dk}{(2\pi)^3} \frac{k^2}{2m} f_1 + \frac{1}{2} \sum_{a,b} \int \frac{dk dp}{(2\pi)^6} T_{ab}(\varepsilon_1 + \varepsilon_2, k, p, 0) f_1 f_2,$$

$$J_{ij}^{\text{qp}} = \sum_a \int \frac{dk}{(2\pi)^3} \left( k_j \frac{\partial \varepsilon_1}{\partial k_i} + \delta_{ij} \varepsilon_1 \right) f_1 - \delta_{ij} E_{\text{qp}},$$

$$n_{a}\text{_{qp}} = \int \frac{dk}{(2\pi)^3} f_1,$$  \hspace{1cm} (12)

and the $\Delta$-contribution following from the scattering integral

$$\Delta E = \frac{1}{2} \sum_{a,b} \int \frac{dk dp dq}{(2\pi)^9} P(\varepsilon_1 + \varepsilon_2) \Delta t,$$

$$\Delta J_{ij} = \frac{1}{2} \sum_{a,b} \int \frac{dk dp dq}{(2\pi)^9} P [(p+q)_i \Delta_{4j} + (k-q)_j \Delta_{3j} - p_i \Delta_{2j}],$$

$$\Delta n_a = \sum_b \int \frac{dk dp dq}{(2\pi)^9} P \Delta t,$$  \hspace{1cm} (13)

where $P = |T_{ab}|^2 2\pi \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) f_1 f_2 (1 - f_3 - f_4)$. The arguments denoted by numerical subscripts are identical to those used in (1), for all $\Delta$'s are explicit.

The density of energy $E = E_{\text{qp}} + \Delta E$ alternatively results from Kadanoff and Baym formula,

$$E = \sum_a \int \frac{dk}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{\omega + \frac{k^2}{2m}}{2} G_a^<(\omega, k, r, t),$$

with $G^<$ in the extended quasiparticle approximation (9). Its complicated form, however, shows that $E$ cannot be easily inferred from an eventual experimental fit of the kinetic equation as it has been attempted in [1]. The conservation of $E$ generalizes the result of Bornath, Kremp, Kraeft and Schlanges [13] restricted to non-degenerated systems. The particle density $n_a = n_{a}\text{_{qp}} + \Delta n_a$ is also obtained from (9) via the definition, $n_a = \int \frac{d\omega}{2\pi} \frac{dk}{(2\pi)^3} G^<$. This confirms that the extended quasiparticle approximation is thermodynamically consistent with the nonlocal and noninstantaneous corrections to the scattering integral.

For equilibrium distributions, formulas (12) and (13) provide equations of state. Two known cases are worth to compare. First, the particle density $n_a = n_{a}\text{_{qp}} + \Delta n_a$ is identical to the quantum
Beth-Uhlenbeck equation of state [3, 13, 16], where \( n_{qp} \) is called the free density and \( \Delta n_a \) the correlated density. Second, the virial correction to the stress tensor has a form of the collision flux contribution known in the theory of moderately dense gases [2, 3].

5 Summary

In this paper we have discussed the kinetic equation which is consistent with thermodynamic observables up to the second order virial coefficient. This theory extends the theory of quantum gases and non-ideal plasma to degenerated systems. The amplitude of the contribution of the off-shell motion is demonstrated on the Wigner distribution which also shows the precision of the extended quasiparticle approximation. The contribution of the nonlocal corrections to the scattering integral is documented on a realistic study of the heavy ion collision within the quantum molecular dynamics. It should be noted, however, that the separable Paris potential used in the presented preliminary results is not fully reliable as seen from comparison of the collision delay and the hard core displacement. Nevertheless, this preliminary study shows that the nonlocal corrections can be evaluated from the T-matrix and incorporated into existing Monte Carlo simulation codes.

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