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Quasiparticle Boltzmann Equation for Nonlocal Binary Collisons

K. MORAWETZ (a), V. ŠPIČKA (b), P. LIPAVSKÝ (b)

(a) Fachbereich Physik, Universität Rostock, 18051 Rostock, Germany
(b) Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16200 Praha 6, Czech Republic

Abstract

Virial corrections to the Boltzmann equation for quasiparticles are obtained from non-equilibrium Green's functions. These corrections are expressed in terms of shifts in space and time that characterize non-locality of scattering integrals. The space shifts parallel finite-diameter corrections to collisions of hard spheres. The time shift is identified as the collision delay. All shifts are given by derivatives of the phase shift in a binary collision.

1 Introduction

The very basic idea of the Boltzmann equation (BE), to balance the drift of particles with dissipation, is used for the description of transport properties of gases, plasmas and condensed systems like metals or nuclei. In all these fields, the BE allows for a number of improvements which make it possible to describe phenomena beyond the range of validity of the original BE. In these improvements theory of gases differs from theory of condensed systems. Two principal streams of kinetic theory are thus established.

In theory of gases, the focus was on so called virial corrections that take into account a finite volume of molecules. The BE includes a contradiction: the scattering cross sections reflect the finite volume of molecules, while the instant and local approximation of scattering events implies the equation of state of an ideal gas. To achieve consistency and extend validity of the BE to moderately dense gases, space non-locality of binary collisions have to be taken into account as it was firstly demonstrated in Enskog's equation [1].

In the theory of condensed systems, modifications of the BE are determined by the quantum mechanical statistics. A headway in this field is covered by the Landau concept of quasiparticles [2]. There are three major modifications: the Pauli blocking of scattering channels; underlying quantum mechanical dynamics of collisions; and quasiparticle renormalization of a single-particle-like dispersion relation. With all these deep modifications, the scattering integrals of the BE remain local in space and time. In other words, the Landau theory does not include a quantum mechanical analogy of virial corrections.

The aim of this article is to bridge these two streams of the kinetic theory. We follow the work [3] where the way how to derive the quasiparticle kinetic equation with nonlocal and noninstant kinetic equation is presented.

2 Kinetic equation

To motivate our approach, let us inspect how the Landau theory exploits information accessible from microscopic theory of binary collisions. Amplitudes of the wave function in individual scattering channels furnishes us with differential cross sections. Phase shifts in the non-dissipative (elastic zero-angle) scattering channel provides the quasiparticle renor-

malization. The information left aside are phase shifts in individual (dissipative) scattering channels.

Already in 1950's, an energy derivative of the phase shift has been identified as a collision delay which naturally measures time non-locality of collisions. Recently, Danielewicz and Pratt [4] pointed out that the collision delay can be used as a convenient tool to introduce virial corrections to the equation of state for the gas of quasiparticles. Although in [4] only equilibrium is discussed, this approach marks a way how to introduce virial corrections also to transport. Of course, out of equilibrium one has to extend their approach to comply with gauge invariance of the system. For instance, the time non-locality has to be accompanied with the space non-locality and the energy and momentum conservation looses its simple form since an external field can drive particles during the collision. Such an extension requires for a systematic approach of rather a general character. To derive the kinetic equation, where collision delays and nonlocalities are expressed via phase shifts, work [3] follows Baerwinkel [5] in starting from nonequilibrium Green's functions and keeping all linear gradient contributions to the scattering integral. Baerwinkel's results are limited to low densities (without medium effects on binary collisions). Instead of the quasiparticle approximation, in [3] the extended quasiparticle approximation [6, 7] is used. This extension is sufficient to gain consistency of the kinetic theory with the virial corrections to thermodynamic quantities.

The derivation of the nonlocal kinetic equation starts from the transport equation first obtained by Kadanoff and Baym [8], $[G_0^{-1} - \Sigma, G^<] + [G, \Sigma^<] = \{G^>, \Sigma^<\} - \{G^<, \Sigma^>\}$, $G^<$ and $G^>$ are particle and hole correlation functions, $G = \frac{1}{2}(G_R + G_A)$ is the hermitian part of the propagator, Σ's are corresponding parts of the selfenergy, and $[A, B] = -i(AB - BA)$ and $\{A, B\} = \frac{1}{2}(AB + BA)$. The self-energy is constructed from the two-particle T-matrix T^R as $\Sigma^<(1,2) = T^R T^A G^> G^< G^<$, (the Bethe-Goldstone approximation [8, 9]), $\Sigma^>$ is obtained by an interchange $> \leftrightarrow <$. This selfenergy is then substituted into the left hand side of the Kadanoff and Baym equation. We want to arrive at the kinetic equation which gives in the classical limit for hard spheres the Enskog equation. To this end, as discussed in [10], using the optical theorem we have to convert the left hand side of the Kadanoff and Baym equation into the form, which is the Green's function precursor of the quantum version of the Enskog equation. Following the approach in [3], the quasiclassical and the extended quasiparticle approximation (1) is then applied.

The extended quasiparticle approximation, derived as the limit of small scattering rates [6, 7],

$$G^{\gtrless}_{1,\omega} = \begin{pmatrix} 1-f_1 \\ f_1 \end{pmatrix} 2\pi z_1 \delta(\omega - \varepsilon_1) + \mathrm{Re}\frac{\Sigma^{\gtrless}_{1,\omega}}{(\omega - \varepsilon_1 - i0)^2}, \tag{1}$$

where $G_{1,\omega} \equiv G_a(\omega, k, r, t)$ and similarly Σ, $z_1 = 1 + \frac{\partial}{\partial\omega}\mathrm{Re}\Sigma_{1\omega}\big|_{\varepsilon_1}$ and the quasiparticle energy ε_1 enables one to convert functional $\Sigma[G]$ to the functional of the quasiparticle distribution $\Sigma[f]$. The first term in (1) brings the on-shell quasiparticle part, the second term is the off-shell contribution.

In contrast to common approach to the quasiclassical approximation of the Kadanoff and Baym equation, here are two essential differences which enables one to arrive at nonlocal kinetic equations. First, we keep all terms linear in gradients in the gradient expansion of the selfenergy. These gradient terms are analogous to those found within the chemical physics [11], where nonlocal kinetic equation was suggested for nondegenerate systems. Second, as shown in [3], nonlocal corrections in the gradient form are not the last step as in [11]. All these terms can be recollected into a nonlocal and noninstant scattering integral, where all nonlocal corrections result proportional to derivatives of the scattering phase shift. The resulting nonlocal kinetic equation reads

$$\frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} =$$

$$= \int \frac{dpdq}{(2\pi)^5}\delta\left(\varepsilon_1+\varepsilon_2^- - \varepsilon_3^- - \varepsilon_4^- - 2\Delta_E\right) z_1 z_2^- z_3^- z_4^- \left(1 - \frac{1}{2}\frac{\partial\Delta_2}{\partial r} - \frac{\partial\varepsilon_2^-}{\partial r}\frac{\partial\Delta_2}{\partial\omega}\right)$$
$$\times|T|^2\left(\varepsilon_1+\varepsilon_2^- - \Delta_E, k-\frac{\Delta_K}{2}, p-\frac{\Delta_K}{2}, q, r-\Delta_r, t-\frac{\Delta_t}{2}\right) f_3^- f_4^-(1-f_1-f_2^-)$$
$$- \int \frac{dpdq}{(2\pi)^5}\delta\left(\varepsilon_1+\varepsilon_2^+ - \varepsilon_3^+ - \varepsilon_4^+ + 2\Delta_E\right) z_1 z_2^+ z_3^+ z_4^+ \left(1 + \frac{1}{2}\frac{\partial\Delta_2}{\partial r} + \frac{\partial\varepsilon_2^+}{\partial r}\frac{\partial\Delta_2}{\partial\omega}\right)$$
$$\times|T|^2\left(\varepsilon_1+\varepsilon_2^+ + \Delta_E, k+\frac{\Delta_K}{2}, p+\frac{\Delta_K}{2}, q, r+\Delta_r, t+\frac{\Delta_t}{2}\right)(1-f_3^+ - f_4^+) f_1 f_2^+. \qquad (2)$$

The subscripts denote shifted arguments: $f_1 \equiv f_a(k,r,t)$, $f_2 \equiv f_b(p, r-\Delta_2, t)$, $f_3 \equiv f_a(k-q-\Delta_K, r-\Delta_3, t-\Delta_t)$, and $f_4 \equiv f_b(p+q-\Delta_K, r-\Delta_4, t-\Delta_t)$. The upperscript $+$ $(-)$ means that shifts have $+$ $(-)$ signs. The Δ's are effective shifts and they represent mean values of various nonlocalities of the scattering integral. These shifts enter the scattering integral in the form known from the theory of gases [1, 11], however, the set of shifts is larger due to the medium effects on the binary collision that are dominated by the Pauli blocking of the internal states of the collision. All the shifts are expressed by the derivatives of scattering phase shift, $\phi = \mathrm{Im}\,\ln T_{sc}^R(\Omega, k, p, q, t, r)$,

$$\begin{aligned}
\Delta_t &= \left.\frac{\partial\phi}{\partial\Omega}\right|_{\varepsilon_3+\varepsilon_4} & \Delta_2 &= \left(\frac{\partial\phi}{\partial p} - \frac{\partial\phi}{\partial q} - \frac{\partial\phi}{\partial k}\right)_{\varepsilon_3+\varepsilon_4} \\
\Delta_E &= -\frac{1}{2}\left.\frac{\partial\phi}{\partial t}\right|_{\varepsilon_3+\varepsilon_4} & \Delta_3 &= -\left.\frac{\partial\phi}{\partial k}\right|_{\varepsilon_3+\varepsilon_4} \qquad (3) \\
\Delta_K &= \frac{1}{2}\left.\frac{\partial\phi}{\partial r}\right|_{\varepsilon_3+\varepsilon_4} & \Delta_4 &= -\left(\frac{\partial\phi}{\partial k} + \frac{\partial\phi}{\partial q}\right)_{\varepsilon_3+\varepsilon_4},
\end{aligned}$$

$[\Delta_r = \frac{1}{4}(\Delta_2+\Delta_3+\Delta_4)]$. After derivatives, Δ's are evaluated at the energy shell $\Omega \to \varepsilon_3+\varepsilon_4$.

This kinetic equation is of the Enskog type having reversed signs of non-local corrections in the scattering-out integral in comparison with scattering-in integral. From (2) the Enskog equation emerges as the classical limit in which the Pauli blocking vanishes, $1-f \to 1$. The hard-sphere potential gives no renormalization of the energy, $\varepsilon_1 \to \frac{k^2}{2m}$, and a phase shift, $\phi = |q|d$, which yields $\Delta_2 = \Delta_4 = \frac{q}{|q|}d$ and all other Δ's are zero.

3 Observables

From definition, all single-particle observables can be expressed in terms of the single-particle density matrix ρ. For instance, the particle density reads $n_a(r,t) = (2\pi)^{-3}\int dk\rho(k,r,t,a)$ and the current density is $j_a(r,t) = -\frac{e}{m}(2\pi)^{-3}\int dk k\rho(k,r,t,a)$. For dilute gases, where the classical BE applies, the single-particle density matrix equals the distribution, $\rho = f$. In dense gases or in condensed matter $\rho \neq f$. This difference is projected onto observables, e.g., $n_a(r,t) \neq (2\pi)^{-3}\int dk f(k,r,t,a)$ in dense gases because of the so called correlated density, and $j_a(r,t) \neq -\frac{e}{m}(2\pi)^{-3}\int dk k f(k,r,t,a)$ in condensed matter because of back-flows. Observables compatible with the transport equation (2) include both kinds of corrections [3].

To identify particle and current densities one can integrate the transport equation (2) over momentum and compare the result with the equation of continuity $\frac{\partial n}{\partial t} + \frac{\partial j}{\partial r} = 0$. An alternative approach is to construct observables directly from Green's functions, $\rho(k,r,t,a) = (2\pi)^{-1}\int d\omega G^<(\omega,k,r,t,a)$, using approximations compatible with those used to derive equation (2), for which end we must use the extended quasiparticle approximation (1) to get the

single-particle density matrix compatible with the transport equation (2)

$$\rho = f - \int \frac{d\omega}{2\pi} \frac{\wp}{\omega - \varepsilon} \frac{\partial}{\partial \omega} \left[f\Sigma_\omega^> - (1-f)\Sigma_\omega^< \right]. \tag{4}$$

Using the quasiparticle approximation for $\Sigma^{>,<}$, one obtains the desired functional $\rho[f]$. Observables like the particle density evaluated from (4) are the same as obtained from the equation of continuity [3]. Of special importance is the local energy conservation which has been proven for degenerate systems [12] in generalization to [7].

4 Summary

We have derived the Enskog -like transport equation for quasiparticles that includes virial corrections to scattering integrals via set of shifts in time, space, momentum and energy. This equation bridges the theory of dense gases and condensed matter. Indeed, neglecting nonlocalities the Landau-Boltzmann transport equation is recovered. The classical Enskog equation results in the classical hard sphere limit. The presented theory is limited to the second virial coefficient by two reasons. First, we have included only binary collisions. Second, the transport equation (2) and the relation (1) has been derived in the limit of small scattering rates [6]. Thus the theory applies to quantum systems with moderately strong interaction: strong enough to be out of scope of the weak coupling limit — weak enough not to destroy quasiparticle picture.

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