A note on binary quantum collision operators conserving mass momentum and energy

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Abstract. In this note, we generalize the Boltzmann collision operator modeling binary particle - particle collisions to a quantum framework using non - local quantum entropy principles.

1 Introduction

This paper is concerned with the derivation of collision operators for the quantum Boltzmann equation

$$\partial_t w + \frac{1}{m_*}\nabla_x \cdot (wp) - \frac{i}{\hbar}\sum_{\sigma=\pm 1} \sigma V(r + \frac{\sigma\hbar}{2i}\nabla_p, t)w = q(w,w) \quad , \tag{1}$$

where $w(x,r,t)$ denotes the Wigner function of a mixed quantum state, $r \in \mathbb{R}^3$ denotes position and $p \in \mathbb{R}^3$ denotes momentum. The function $V(r,t)$ denotes the potential and the operator $V(r + \frac{\sigma\hbar}{2i}\nabla_p, t)$ in (1) is understood in the sense of pseudo differential operators [8]. $q(w,w)$ is a bilinear operator modeling binary collisions between particles. The Wigner equation (1) is obtained from the Heisenberg equation for the density matrix $\rho(x,y,t)$

$$i\hbar\partial_t \rho = [H,\rho] + i\hbar Q(\rho,\rho) \quad , \tag{2}$$

where $[H,\rho]$ denotes the usual commutator of ρ with the Hamiltonian $H = -\frac{\hbar^2}{2m_*}\Delta + V$, through the Wigner - Weyl transform

$$w = W[\rho](r,p,t) = (2\pi)^{-3}\int \rho(r - \frac{\hbar}{2}\eta, r + \frac{\hbar}{2}\eta, t)\exp(i\eta\cdot p)d\eta \quad . \tag{3}$$

The form of the collision operator Q, which is related to q in the Wigner picture (1) via $q(W[\rho],W[\rho]) = W[Q(\rho,\rho)]$, is the subject of this paper. Various approaches exist to modeling collisions of particles with a background in a quantum mechanical framework [1], [2],[3],[7] . Since they model collisions with a background they result in linear collision operators. We, on the other hand, are concerned with particle - particle collisions, and therefore the collision operators in (1) and (2) have to be nonlinear. In analogy to the classical case, we will derive the general form of the collision operator q from two requirements, namely

Work supported by NSF award DECS-0218008

- $q(w,w)$ locally conserves a given set of quantities $\kappa_m(p),\ m = 0,..,M$, where we always assume $\kappa_0(p) = 1$, i.e. we assume at least mass conservation.
- $q(w,w)$, or in the density matrix picture (2) $Q(\rho,\rho)$, dissipates the logarithmic quantum entropy.

Based on these two assumptions we can derive the form of $Q(\rho,\rho)$. The derivation is analogous to the one leading to the classical Boltzmann operator [4], except that the quantum entropy is defined as a global quantity, namely the trace of an operator, instead of the simple logarithm of the density function.

2 The quantum collision operator

In this section we derive the form of the collision operator from the two requirements above. The way the local conservation properties are used in Section 2.1 is precisely the same as for the classical Boltzmann collision operator and can be found c.f. in [4]. The quantum nature of the collision operator enters through the use of the quantum entropy in Section 2.2

2.1 Conserved quantities

We start by using the assumption that $q(w,w)$ locally conserves mass, i.e. $\kappa_0 = 1$ holds, or

$$\int q(w,w)(r,p,t)\ dp = 0, \quad \forall w,r,t$$

holds. This implies that we can write the collision operator q in weak form as

$$\int \phi(p)q(w,w)(r,p,t)\ dp = \tag{4}$$

$$\frac{1}{2}\int K(w,w,t,r,p,p_1,p',p_1')[\phi(p')+\phi(p_1')-\phi(p)-\phi(p_1)]\ dpdp_1dp'dp_1' \quad ,$$

for any test function $\phi(p)$, where K is an operator acting on the Wigner function w satisfying the symmetry relations

$$K(w,w,t,r,p,p_1,p',p_1') = K(w,w,t,r,p_1,p,p_1',p') \quad . \tag{5}$$

Clearly, the form (4) implies local mass conservation since the integral vanishes for constant test functions ϕ. On the other hand, any mass conserving operator q can be trivially written in the form (4). Next we use the additional conservation properties, i.e. the integral in (4) has to vanish for all Wigner functions w when choosing $\kappa_m, m = 1,..,M$ as test functions. So

$$\int K(w,w,t,r,p,p_1,p',p_1')[\kappa_m(p')+\kappa_m(p_1')-\kappa_m(p)-\kappa_m(p_1)]\ dpdp_1dp'dp_1' = 0,$$

$$m = 1,..,M, \quad \forall w,r,t \quad ,$$

has to hold. Note, that the index m only ranges from $m = 1,..,M$ since $\kappa_0 = 1$ is automatically conserved by writing q in the form (4). This implies that K is supported only on the set of

p, p_1, p', p'_1 for which $\kappa_m(p') + \kappa_m(p'_1) - \kappa_m(p) - \kappa_m(p_1) = 0$ holds for $m = 1, .., M$. Therefore we can write

$$K(w, w, t, r, p, p_1, p', p'_1) = K_1(w, w, t, r, p, p_1, p', p'_1) \prod_{m=1}^{M} \delta(\kappa_m(p') + \kappa_m(p'_1) - \kappa_m(p) - \kappa_m(p_1)) \quad , \tag{6}$$

where the operator K_1 satisfies the same symmetry relations (5) as K. Usually, momentum and energy will be conserved in addition to mass. So $M = 2, \kappa_1(p) = p, \kappa_2(p) = \frac{|p|^2}{2m_*}$ will hold.

2.2 Dissipation of the logarithmic quantum entropy

As an additional requirement we impose that the operator Q in the Heisenberg equation (2) dissipates the quantum entropy [9], i.e. that

$$Tr[\ln_M(\rho)Q(\rho, \rho)] \leq 0 \quad \forall \rho$$

holds for all density matrices ρ. Here, we denote by $\ln_M(\rho)$ the logarithm of a selfadjoint operator (or density matrix), defined in the usual way via its spectral decomposition. The symbol Tr denotes the trace of the operator, so $Tr[\rho_1\rho_2] = \int \rho_1(x, y)\rho_2(y, x)\ dxdy$ holds. A direct calculation, using the definition (3) of the Wigner transform, yields that the trace of the product of two density matrices translates in the Wigner picture to

$$Tr[\rho_1\rho_2] = \int W[\rho_1](r, p, t)W[\rho_2](r, p, t)\ drdp \quad .$$

Thus, we require that

$$\int W[\ln_M(\rho)]q(w, w)\ drdp \leq 0$$

holds for all density matrices ρ with $w = W[\rho]$. Note, that, other than in the classical case, the entropy is a global quantity. Using the weak formulation (4) of the collision operator q this gives

$$\int K(w, w, t, r, p, p_1, p', p'_1)(f' + f'_1 - f - f_1)\ drdpdp_1dp'dp'_1 \leq 0, \quad f = W[\ln_M(\rho)], \quad w = W(\rho) \quad , \tag{7}$$

where we write, for short $f' = f(r, p', t), f_1 = f(r, p_1, t)$ and so on. In analogy to the classical case, we write the operator K in (4) as

$$K(w, w, t, r, p, p_1, p', p'_1) = A[w](r, p, t)A[w](r, p_1, t)S(r, p, p_1, p', p'_1)$$

with A some operator acting on the Wigner function w and the scattering cross section S satisfying the symmetry conditions

$$S(r, p, p_1, p', p'_1) = S(r, p_1, p, p'_1, p') = S(r, p', p'_1, p, p_1) \quad . \tag{8}$$

In addition, because of the conservation properties discussed in 2.1, the scattering cross section S has to be of the form

$$S(r, p, p_1, p', p'_1) = S_1(r, p, p_1, p', p'_1) \prod_{m=1}^{M} \delta(\kappa_m(p') + \kappa_m(p'_1) - \kappa_m(p) - \kappa_m(p_1)) \quad , \tag{9}$$

in order to satisfy (6). The additional symmetry of S in (8) allows us to write (7) as

$$\frac{1}{2}\int (gg_1 - g'g'_1)S(r,p,p_1,p',p'_1)(f'+f'_1-f-f_1)\ drdpdp_1dp'dp'_1 \leq 0, \tag{10}$$

$$g = A[w], \quad f = W[\ln_M(\rho)], \quad w = W(\rho) \quad .$$

Assuming that the scattering cross section S_1 is strictly positive, the inequality (10) can now be achieved by setting $g = e^f$ or $A[W[\rho]] = e^{W[\ln_M(\rho)]}$. This gives for the collision operator $q(w,w)$ in its strong formulation

$$q(w,w)(r,p,t) = \int S(r,p,p_1,p',p'_1)(g_1g'_1 - gg_1)\ dp'dp'_1dp_1, \quad g(r,p,t) = e^{W[\ln_M(W^{-1}[w])]} \tag{11}$$

where the inverse Wigner transform W^{-1} is given by

$$W^{-1}[w](x,y,t) = \int w(\frac{x+y}{2},p,t)\exp[\frac{i}{\hbar}p\cdot(x-y)]\ dp \quad , \tag{12}$$

And the kernel S is given by (9) with some scattering cross section S_1. Note, that the exponential function in (11) is the usual exponential function while the logarithm is the logarithm of an operator.

3 Equilibria and local Maxwellians

We now investigate the kernel of the collision operator $q(w,w)$, given in (11). If the density matrix ρ_0 is such that $q(w_0,w_0)=0$ holds for $w_0 = W[\rho_0]$, then obviously

$$\int W[\ln_M(\rho_0)]q(w_0,w_0)\ drdp = 0$$

holds as well. In this case, using (10), we obtain

$$\frac{1}{2}\int (gg_1 - g'g'_1)S(r,p,p_1,p',p'_1)(f'+f'_1-f-f_1)\ dpdp_1dp'dp'_1 = 0$$

$$\text{with } g = e^{W[\ln_M(\rho_0)]}, \quad f = W[\ln_M(\rho_0)] = \ln(g) \quad .$$

Using the form (9) of the scattering cross section S, and the fact that $S_1 > 0$, holds we obtain

$$(e^{f'+f'_1} - e^{f+f_1})(f'+f'_1-f-f_1)\prod_{m=1}^{M}\delta(\kappa_m(p')+\kappa_m(p'_1)-\kappa_m(p)-\kappa_m(p_1)) = 0 \quad \forall p,p_1,p',p'_1 \quad .$$

This implies that f is a linear combination of the quantities $\kappa_m(p),\ m = 0,..,M$ with coefficients which can depend on the position r and the time t. $\kappa_0(p) = 1$ can be included in this linear combination. Thus, we obtain

$$f(r,p,t) = \sum_{m=0}^{M} a_m(r,t)\kappa_m(p), \text{ and } \rho_0 = \exp_M(W^{-1}[f]), \quad w_0 = W[\exp_M(W^{-1}[f])], \tag{13}$$

for the equilibrium density matrix and Wigner function ρ_0 and w_0. On the other hand, a Wigner function of the form (13) clearly is in the kernel of the operator q defined by (11), and therefore the kernel of q consists precisely of Wigner functions of the form (13). Here $\exp_M$ denotes the matrix exponential defined via the spectral decomposition of ρ and W and W^{-1} are defined by (3) and (12) respectively. (13) is the quantum equivalent of the classical local Maxwellian and has been used in [5],[6] for the derivation of hydrodynamic closures of the quantum Boltzmann equation.

4 Conclusions

Based on the assumptions that binary collisions locally conserve a given set of quantities and dissipate the global logarithmic quantum entropy, we have derived a quantum version of the Boltzmann collision operator. The non - local nature of quantum collisions is reflected by the fact that, although its conservation properties are local, the operator itself is spatially non - local because of the operator logarithm in (11). The quantum collision operator will reduce to the usual Boltzmann operator in the classical limit, since the operator $A[w] = e^{W[\ln_M(W^{-1}[w])]}$ can be expected to reduce to the identity in this limit.

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