Comment on "Quantum linear Boltzmann equation with finite intercollision time"

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Inconsistencies are pointed out in a recent proposal [L. Diósi, Phys. Rev. A **80**, 064104 (2009)] for a quantum version of the classical linear Boltzmann equation.

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I. INTRODUCTION

In a recent Brief Report [1] Diósi proposes a quantum version of the classical linear Boltzmann equation. As explained below, we think that this proposed equation has a number of unfavorable properties, both from a physical and from a conceptual point of view, which cast serious doubts on its validity. All these problems are nonexistent in what we consider the appropriate quantum linear Boltzmann equation (QLBE) [2–4], while the proposed equation has no physically meaningful advantage over the QLBE. In particular, the possible wish for linearity in the gas momentum distribution, which serves as the motivation of [1], is consistently fulfilled within the QLBE by an approximation that is much less drastic than the modifications entailed in [1].

We are concerned with a Markovian quantum master equation for the motion of a single, distinguished test particle (mass M) due to collisions with a stationary, homogeneous, and ideal background gas of distinguishable particles (mass m, density $n_{\rm gas}$). The latter is characterized by the momentum distribution function $\mu_{\rm gas}(\boldsymbol{p}) = \langle \boldsymbol{p}|\rho_{\rm gas}|\boldsymbol{p}\rangle$, which may or may not be given by the Maxwell distribution. The equation is supposed to be valid as long as a Markovian description of the reduced quantum state of the test particle is appropriate.

II. DISCUSSION OF THE MASTER EQUATION

Diósi's proposal involves an "intercollision time"

$$\tau = \frac{1}{n_{\rm gas}\sigma}\sqrt{\frac{\pi m}{k_{\rm B}T}}, \tag{1}$$

and his master equation is constructed such that in the limit of vanishing gas density $n_{\rm gas} \to 0$, i.e., for $\tau \to \infty$, it reduces to the classical linear Boltzmann equation for the diagonal momentum matrix elements. In the following, we do not discuss our reservations about the derivation of the proposed equation and the implied violation of energy conservation in individual scattering interactions, but we consider only problems of the final master equation at finite τ. We start by exposing conceptual deficiencies and then move on to inconsistencies in the predicted physical behavior.

A. Conceptual deficiencies

1. Off-shell extension ill defined

The equation is not well defined because it involves the elastic scattering amplitude $f(\boldsymbol{p}_f, \boldsymbol{p}_i)$ at off-shell values $|\boldsymbol{p}_i| \neq |\boldsymbol{p}_f|$. While it is common in scattering theory to work with off-shell extensions of the scattering operators, this is only done for computational convenience [5]. All physically relevant properties of the elastic scattering process depend solely on the on-shell values, not least because of the arbitrariness of the off-shell extension [5]. Even if one were to agree on a definite choice of the off-shell extension, the proposed equation would remain ill defined because the value of the off-shell energy parameter, which is an independent variable, remains unspecified.

From a physical point of view, it seems implausible that the supposed "energy uncertainty" related to finite intercollision times (a property involving the state of motion of gas and test particle) has anything to do with a possible off-shell extension of the elastic scattering amplitude (which is a function of the interaction potential only).

2. Dependence on representation of δ function

The proposed equation depends on a particular choice of the representation of the δ function. It has the property that its square can be related to another representation of the δ function. One can envisage representations of the δ function quite different from the one used in the proposed equation, which share the same property, e.g., a Gaussian function. Those would yield manifestly different equations (e.g., leading to a different prediction for the constant D_{xx}). This highlights the arbitrariness of using a particular representation. From a physical point of view, it seems implausible that one form of "smoothing" should be favored over another.

3. Nonlinearity in the gas density

The proposed equation is nonlinear with respect to the gas density since the definition (1) of τ includes $n_{\rm gas}$. From a physical point of view, it seems implausible that the Liouvillian for the Markovian dynamics should be a nonlinear function of $n_{\rm gas}$. The reason is that the background gas is noninteracting and nondegenerate, implying that the gas particles are uncorrelated, while three-particle collisions are excluded by assumption. Therefore, each gas particle affects the test particle equally, so that its effect is described by the same mapping. This implies that the Liouvillian for the effect of the total gas is proportional to the number of gas particles, rendering the master equation linear in $n_{\rm gas}$.

4. Definition of τ

If the quantity τ is to correctly describe the time elapsing between collisions among gas and test particle, it should not

depend only on the state of the gas [via the temperature in (1) or more generally via $\mu_{\rm gas}(\boldsymbol{p}) = \langle \boldsymbol{p}|\rho_{\rm gas}|\boldsymbol{p}\rangle$], but it must also depend on the motional state of the test particle. The definition (1) is therefore inappropriate, in particular if the test particle is much faster than the gas particles. In addition, (1) is not well defined because the energy dependence of $\sigma_{\rm tot}$ is not specified. The physically meaningful mean intercollision time is given by the expression [6]

$$\tau_{\rm phys}^{-1}[\rho] = \int d\boldsymbol{P}\langle \boldsymbol{P}|\rho|\boldsymbol{P}\rangle n_{\rm gas} \int d\boldsymbol{p}\mu_{\rm gas}(\boldsymbol{p}) \times v_{\rm rel}(\boldsymbol{p},\boldsymbol{P})\sigma_{\rm tot}\big[E_{\rm rel} = m_* v_{\rm rel}^2(\boldsymbol{p},\boldsymbol{P})/2\big], \quad (2)$$

with $v_{\rm rel}(\boldsymbol{p},\boldsymbol{P}) = |\boldsymbol{p}/m - \boldsymbol{P}/M|$ the relative velocity, and m_* the reduced mass. However, the use of the appropriate definition (2) in [1] would yield a nonlinear time evolution equation for ρ, thus violating the basic requirement of a linear quantum state evolution.

From a physical point of view, the dependence of the collision rate on the state of the test particle is rather important, not least because the total cross section may depend strongly on $E_{\rm rel}$ for large test particle velocities. Moreover, this dependence is necessary to grant the approach to the stationary solution. We note that the QLBE discussed in [2–4] incorporates this dependence of the collision rate on ρ [by means of a rate operator with expectation value $\tau_{\rm phys}^{-1}[\rho]$; see Eq. (12) in [3]], while the required linearity in ρ is a result of the use of concepts from the theory of generalized quantum measurements [7].

5. Dynamics of momentum populations

As a natural consistency requirement, one expects that once the test particle state is indistinguishable from a classical phase space distribution, its dynamics should be governed by the classical linear Boltzmann equation (with a quantum mechanical scattering cross section). This is not fulfilled in the proposed equation since at finite $n_{\rm gas}$ the dynamics of the populations in the momentum representation differs from the one predicted by the classical equation, implying a discontinuous transition to the classical description at a finite gas density.

6. No canonical stationary solution

As a consequence of Sec. II A 5, the canonical thermal state of the test particle, $\rho \propto \exp(-\beta \mathsf{P}^2/2M)$, is not a stationary solution of the proposed master equation in a Maxwell-Boltzmann gas. In particular, the collision kernel does not satisfy the detailed balance condition. From a physical point of view, it seems quite important that the state of maximal entropy corresponds to the stationary solution. This is the case even in extensions of the QLBE which account for quantum degeneracies in the gas [4].

7. Infinite "position diffusion" for $n_{\rm gas} \to 0$

The limit of quantum Brownian motion of the proposed master equation predicts a "position diffusion" coefficient D_{xx} [given in Eq. (23) of [1]] that grows above all bounds as one decreases the gas density $n_{\rm gas} \to 0$. However, one expects the free Schrödinger equation to be obtained in the limit of vanishing gas density, so that the predicted behavior is obviously unphysical.

B. Supposed linearity in the gas momentum distribution

Let us now comment on the supposed linearity in the gas momentum distribution discussed in [1]. First, we note that (1) is a function of the gas temperature and therefore in general a functional of the gas momentum distribution, $\tau = \tau[\mu_{\rm gas}]$. Writing the gas state dependence of the proposed equation in a consistent fashion, one thus finds that the proposed equation is a manifestly nonlinear expression in $\mu_{\rm gas}$, in stark contrast to the claim in [1]. The advertised advantage of the proposed equation is therefore unfulfilled.

At the same time, it seems doubtful whether one can or should expect linearity in $\mu_{\rm gas}$ within a Markovian description. A linear behavior of the reduced time evolution with respect to an initial, uncorrelated $\rho_{\rm gas}(0)$ can be expected only based on an exact solution for system plus environment, while a Markovian description necessarily involves approximations, required to obtain a Lindblad structure of the generator, granting complete positivity of the quantum evolution [8]. The linearity in $\mu_{\rm gas}$ is recovered easily in the framework of the QLBE once the test particle momentum operator can be approximated by a characteristic $\mathbb{C}$-number in the argument of $\mu_{\rm gas}$.

C. Momentum decoherence

We now consider the "apparently overlooked" "surprising collisional decoherence effect" advocated in [1]. It is important to stress that, far from being overlooked, the effect of the momentum exchange due to a single collision is fully accounted for in the QLBE, as already discussed in [4,9,10]. The decoherence rate for a hypothetical superposition of two different momentum states is predicted by the QLBE to be the average of the corresponding total collision rates. This is indeed required on physical grounds since any collision changes the momentum by definition, and it is immediately seen by looking at the momentum representation of the equation, Eq. (2.7) in [4]: Considering the off-diagonal element that characterizes the coherence, one notes that the "gain terms" do not affect its temporal change because for an initial superposition of momentum eigenstates there are no other off-diagonal elements, so that the initial decoherence rate is given by the "loss terms" arising from the anticommutator, which amount to the arithmetic mean of the total collision rates. Since there are no stronger physical decoherence mechanisms available, we consider any prediction beyond this as unphysical.

We emphasize that the detailed derivation of the QLBE applies dynamic scattering theory to a wave packet decomposition of the relative motion [3]. As such, all the details of the dynamic quantum scattering process are incorporated by construction, including the particles' energy uncertainty and the finite interaction time. There is no room for additional effects in the framework of the two-particle Schrödinger equation. The limits of this treatment are met precisely if the test particle can never be considered asymptotically free between two collisions because it interacts with more than one gas particle all the time. The notion of an intercollision time is meaningless in such situations, and it would be wrong to use scattering theory altogether.

D. Non-Markovian extensions

As for non-Markovian extensions, it is clear that the QLBE loses its validity at densities and temperatures where the collisions can no longer be taken as independent two-particle events, since the interactions between the gas particles start to play a role and the collisions cannot be considered as complete. The related problem of the derivation of non-Markovian quantum kinetic equations for the description of self-interacting dense gases has been considered, e.g., in [11,12], relying on advanced many-body techniques. In such frameworks non-Markovian quantum extensions of the nonlinear Boltzmann equation have been obtained, indicating that memory effects in dense gases beyond the Born approximation generally involve nontrivial memory kernels. The difficulties listed above in Secs. II A 1–II A 7 might be avoidable by pursuing an analogous microscopic approach for the QLBE, rather than introducing arbitrary *ad hoc* modifications. It thus appears that entirely new theoretical approaches are required at high densities, not least since non-Markovian effects or corrections cannot possibly be described by a master equation in Lindblad form with time-independent coefficients [13]. In any case, it seems reasonable to use the properties of the QLBE, including its various limiting forms and its experimental confirmations discussed in [4], as a benchmark consistency check for any proposed extension of that master equation.

III. CONCLUSION

In summary, the equation proposed in [1] provides no physically meaningful advantage over established results, while displaying conceptual inconsistencies, as well as leading to unphysical predictions. We conclude that, rather than bringing "a dramatic change in our understanding of the quantum behavior of the test particle," the equation in [1] is a step in the wrong direction.

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