Reply to "Comment on 'Generalized exclusion processes: Transport coefficients' "

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We reply to the Comment of Becker, Nelissen, Cleuren, Partoens, and Van den Broeck [Phys. Rev. E **93**, 046101 (2016)] on our article [Arita, Krapivsky, and Mallick, Phys. Rev. E **90**, 052108 (2014)] about the transport properties of a class of generalized exclusion processes.

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Stochastic lattice gases with symmetric hopping are described, on a coarse-grained level, by the diffusion equation with a density-dependent diffusion coefficient. Density fluctuations depend in addition on the local conductivity (which also describes the response to an infinitesimal applied field). A hydrodynamic description, therefore, requires the determination of these two transport coefficients. Generally for lattice gases even with rather simple hopping rules, analytic results are unattainable; however, when an additional feature, known as the *gradient condition*, is satisfied, the Green-Kubo formula takes a simple form [1] and computations of the transport coefficients become feasible. For a number of lattice gases of gradient type, e.g., the Katz-Lebowitz-Spohn model with symmetric hopping [2], the repulsion processes [3], and a lattice gas of leap-frogging particles [4,5], the diffusion coefficient has been rigorously computed. The gradient property is also true for the misanthrope process, a class of generalized exclusion processes [6,7].

For gradient-type lattice gases, an exact expression for the diffusion coefficient can also be obtained by a perturbation approach: one writes the formula for the current at the discrete lattice level and then performs a continuous limit assuming that the density field is slowly varying.

Generalized exclusion processes with multiple occupancies [8–11], in general, do not obey the gradient condition. However, we argued in [12] that the perturbation approach should, nevertheless, lead to an exact prediction for the diffusion coefficient. For the class of generalized exclusion processes that we studied [12], simulation results were indeed very close to the perturbative calculation predictions. The Comment [13] by Becker *et al.* prompted us to perform more simulations and to analyze our results more carefully.

Becker *et al.* computed numerically the diffusion coefficient $D(\rho)$. They performed simulations for various system sizes L and various density differences $\delta\rho$ between the boundary reservoirs. To extract $D(\rho)$ from simulations, they needed to take [13] two limits: $L \to \infty$ and $\delta\rho \to 0$. We considered a system with a large density difference and measured the stationary current through the system: the advantage is that we have to take only one limit, $L \to \infty$. We analyzed the generalized exclusion process GEP(2) with maximal occupancy $k = 2$ particles per site and extreme densities at the boundaries: $\rho(0) = 2$ and $\rho(L) = 0$. According to our expectations [12], the average current should vanish as $(1 + \frac{\pi}{2})/L$ when $L \gg 1$. Simulation results (Fig. 1) demonstrate that the error is smaller than 0.9%, but this discrepancy does not seem to disappear in the $L \to \infty$ limit.

The numerical results of Ref. [13] and our simulations (Fig. 1) show that the perturbation approach does not lead to the correct analytical results for the GEP(2). We emphasize that the perturbation approach is *not* a naive mean-field theory where correlations are obviously neglected, as argued by Becker *et al.* In dense lattice gases, the equilibrium state itself is usually highly correlated. For example, in the repulsion process $\langle \tau_i \tau_{i+1} \rangle = 0 \neq \rho^2$ for $0 \leqslant \rho \leqslant \frac{1}{2}$, where $\tau_i \in \{1,0\}$ denotes the occupation number of site i, the mean-field assumption is completely wrong. Yet, a careful use of the perturbation approach leads to the correct result [3].

The gradient condition is thus crucial for the applicability of the perturbation approach. For GEP(k) with maximal occupancy k, the gradient condition is obeyed in extreme cases of $k = 1$, which reduces to the simple exclusion process, and $k = \infty$, which reduces to random walks. Presumably because GEP(k) is sandwiched between two extreme cases in which the perturbation approach works, this method provides a very good approximation when $1 < k < \infty$.

We now clarify the underlying assumptions behind the perturbation approach and suggest some ways to improve our results. For the GEP(2), the current reads

$$J_i = \langle \tau_i f(\tau_{i+1}) - f(\tau_i)\tau_{i+1} \rangle, \tag{1}$$

where $\tau_i \in \{0,1,2\}$ and $f(n) = 1 - \frac{1}{2}n(n-1)$. In our computation of the diffusion coefficient [12], we used two assumptions. The first one concerns one-point functions. Let $\mathbb{P}[\tau_i = m]$ be the probability of finding m particles at site i. The density at i is

$$\rho_i = \langle \tau_i \rangle = \mathbb{P}[\tau_i = 1] + 2\mathbb{P}[\tau_i = 2]. \tag{2}$$

We assumed that one-site probabilities satisfy

$$\mathbb{P}[\tau_i = m] \simeq X_m(\rho_i), \tag{3}$$

where the X_m's represent the single-site weights in an infinite lattice or on a ring:

$$X_0(\rho) = \frac{1}{Z}, \quad X_1(\rho) = \frac{\lambda}{Z}, \quad X_2(\rho) = \frac{\lambda^2}{2Z} \tag{4}$$

with the fugacity λ and the normalization Z,

$$\lambda(\rho) = \frac{\sqrt{1 + 2\rho - \rho^2} + \rho - 1}{2 - \rho}, \quad Z = 1 + \lambda + \frac{1}{2}\lambda^2. \tag{5}$$

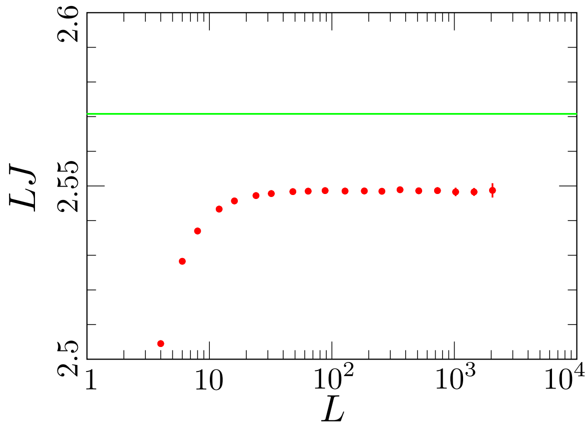

FIG. 1. Stationary current multiplied by the system size: simulation results (dots) and the prediction from our previous approach. The latter holds for $L = \infty$, but is shown as a line.

The second assumption was to rewrite the current as

$$J_i \simeq \langle \tau_i \rangle \langle f(\tau_{i+1}) \rangle - \langle f(\tau_i) \rangle \langle \tau_{i+1} \rangle. \quad (6)$$

This is indeed a mean-field-type assumption [13]. The assumptions (3) and (6) are asymptotically *true* in the stationary state of a large system ($L \to \infty$): We have checked these facts by performing additional simulations.

Our numerical results suggest more precise expressions for (3) and (6) with some scaling functions κ and μ:

$$\mathbb{P}[\tau_i = m] = X_m(\rho_i) + \frac{1}{L}\kappa_m\left(\frac{i}{L}\right), \quad (7)$$

$$J_i = \langle \tau_i \rangle \langle f(\tau_{i+1}) \rangle - \langle f(\tau_i) \rangle \langle \tau_{i+1} \rangle + \frac{1}{L}\mu\left(\frac{i}{L}\right), \quad (8)$$

where we omitted $o(L^{-1})$ terms. Performing the perturbation approach with the refined expressions (7) and (8), we obtain

$$J = -\frac{1}{L}\frac{d\rho}{dx}\left(1 - X_2(\rho) + \rho\frac{dX_2(\rho)}{d\rho}\right) + \frac{1}{L}\mu(x), \quad (9)$$

where we have switched from the discrete variable i to $x = i/L$. The functions κ_m do not appear in (9), but $\mu(x)$ does, and it was missing in our paper [12], leading to the wrong expressions for the current and for the stationary density profile. To calculate $\mu(x)$, we are presently examining nearest-neighbor correlation functions for the GEP(2). Numerically at least, these nearest-neighbor correlations exhibit a neat scaling behavior and simple patterns; detailed results will be reported in [14].

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