Mean-field approach for diffusion of interacting particles

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A nonlinear Fokker-Planck equation is obtained in the continuous limit of a one-dimensional lattice with an energy landscape of wells and barriers. Interaction is possible among particles in the same energy well. A parameter γ, related to the barrier's heights, is introduced. Its value is determinant for the functional dependence of the mobility and diffusion coefficient on particle concentration, but has no influence on the equilibrium solution. A relation between the mean-field potential and the microscopic interaction energy is derived. The results are illustrated with classical particles with interactions that reproduce fermion and boson statistics.

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I. INTRODUCTION

The complete description of a large number of interacting particles (a many-body system) is a problem that usually exceeds numerical or analytical capabilities. Mean-field theory allows the description of such a system by analyzing the behavior of only one particle subjected to an average force produced by the rest of the particles. The mean-field force depends on statistical properties of the rest of the particles that, for self-consistency, are equal to the properties of the particle considered before [1]. This is the origin of the nonlinear character of the resulting description (see [2], p. 3). The nonlinearities reflect the interactions between particles. For example, Kaniadakis and Quarati [3] introduced a nonlinear Fokker-Planck equation for the particle density in a classical system that reproduces quantum statistics. An appropriate choice of the transition probabilities that depend on the particle density gives rise to Fermi-Dirac or Bose-Einstein distributions in equilibrium. Quantum effects can be reproduced in a classical system with an interaction potential, also called a statistical potential [4]. For example, the Pauli exclusion principle for fermions is analogous to a potential that becomes infinite when two particles occupy the same state. This hard-core interaction is the cause of a nonlinear term in the corresponding diffusion equation [see [3]; [2], p. 280; or Eq. (10) in [5]]. A general approach for the derivation of a nonlinear Fokker-Planck equation starting from the master equation can be found in [6,7]. More examples can be found in [2]. Many researchers have devoted attention to the problem of diffusion with interaction, in many cases motivated by the seminal work of Batchelor [8] (see also the related works [9–25]).

The problem that we wish to address, from a quite general perspective, is collective diffusion of interacting particles. We use a one-dimensional lattice, but the results can be easily extended to higher dimensions. In our analysis, only the collective or transport diffusion coefficient is involved (we do not analyze here single-particle diffusion or self-diffusion of tagged particles).

The restriction on the interaction is that it is local: It takes effect only among particles in the same site. In other words, the interaction range is smaller than the lattice spacing. We apply a mean-field approximation assuming that the evolution of the system can be obtained by analyzing the behavior of only one particle. We consider that this particle is subjected to a mean-field potential V_i that depends on the number of particles in the site n_i, where i is the lattice site index. The variation of the particle number is smooth, so the continuous limit can be applied and a nonlinear Fokker-Planck equation is obtained. The equilibrium solution is completely determined by the mean-field interaction potential and, if present, an external potential. This is not the case for the nonequilibrium behavior. As we show in the following sections, it depends on an additional parameter γ that determines if the transition probability between neighboring sites depends on the potential in the source site, in the target site, or on a mixture of both potentials. We also show that this parameter is experimentally accessible through the measurement of the concentration-dependent mobility and diffusion coefficient.

II. TRANSITION PROBABILITIES

In the one-particle picture, the energy associated with a particle in site i is given by

$$E_i = V_i + U_i, \tag{1}$$

where V_i, the internal or mean-field potential, is an abbreviation of $V(n_i)$ and U_i is an external potential. We can consider V_i as a function of n_i that, in equilibrium, satisfies the relation $n_{\mathrm{eq,i}} \propto \exp\{-\beta[V(n_{\mathrm{eq,i}}) + U_i]\}$, i.e., it is a one-particle effective potential that satisfies Boltzmann statistics in equilibrium.

The interaction energy of a configuration of n_i particles is given by a function $\Phi(n_i)$. The relevant problem of determining the relation between the mean-field potential V_i and the interaction energy $\Phi(n_i)$ is addressed in Sec. IV. The interaction is local in the sense that particles interact only when they are at the same site.

In the one-particle picture, the detailed balance condition gives a relation between transition probabilities

$$e^{-\beta E_{i+1}} W_{i+1,i} = e^{-\beta E_i} W_{i,i+1}, \tag{2}$$

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where $W_{i,i+1}$ is the transition probability from site i to site $i+1$. Using the words of Derrida [26], it is a "straightforward generalization" to consider that (2) also holds for the transition probabilities out of equilibrium (it is clear that this does not mean that detailed balance holds out of equilibrium, since in general $n_i \neq \text{const} \times e^{-\beta E_i}$).

Detailed balance is not enough to determine the transition probabilities. In order to obtain an expression for them, we assume that they can be written as a combination of exponentials of V_i, V_{i+1}, U_i, and U_{i+1}. In the following we present a physical interpretation of the result that also serves as a justification of this assumption. We have

$$W_{i,i+1} = P \exp[-\beta(\gamma V_{i+1} + \gamma' V_i + \alpha U_{i+1} + \alpha' U_i)], \quad (3)$$

where γ, γ', α, α', and P may depend on position i; the subindex is omitted in order to simplify the notation. We assume that the system has an inversion symmetry. This implies that the reversed transition probability is obtained from (3) by exchanging $i \leftrightarrow i+1$:

$$W_{i+1,i} = P \exp[-\beta(\gamma V_i + \gamma' V_{i+1} + \alpha U_i + \alpha' U_{i+1})]. \quad (4)$$

It can be shown that the combination that fulfills detailed balance is $\gamma' = \gamma - 1$ and $\alpha' = \alpha - 1$. Then

$$W_{i,i+1} = P e^{-\beta[(\gamma-1)V_i + \gamma V_{i+1} + (\alpha-1)U_i + \alpha U_{i+1}]}. \quad (5)$$

A physical interpretation of the parameters γ and α is related to the barrier's height between neighboring sites. Let us consider that particles can occupy discrete sites in a lattice with a potential that has a continuous shape, as shown in Fig. 1. Between sites i and $i+1$, the potential has a maximum value of $B_{i+1/2}$. A particle that jumps from i to $i+1$ has to overcome a barrier $B_{i+1/2} - E_i$ and the transition probability is given by

$$W_{i,i+1} = \nu e^{-\beta(B_{i+1/2} - E_i)}, \quad (6)$$

where ν is the number of jump attempts per unit time. The potential maxima depend, on the one hand, on the characteristics of the substratum, which contributes with a term C. They also may depend on the values of the interaction potential on both sides of the barrier. This dependence is symmetrical (the same for both sides) and its influence is represented by a term $\gamma(V_i + V_{i+1})$; the choice of the name of the parameter γ advances that it is the same as the one introduced in (5). Finally, the external potential also has an influence on the barriers. It is given by an additional parameter $\eta \in (0,1)$: $\eta U_i + (1-\eta)U_{i+1}$. The influence of the external potential on the barriers is always present. The parameter η is an interpolation factor between sites i and $i+1$ for this influence. Taking these arguments together, the potential maximum is

$$B_{i+1/2} = C + \gamma(V_i + V_{i+1}) + \eta U_i + (1-\eta)U_{i+1}. \quad (7)$$

Substituting in (6) and considering that $P = \nu e^{-\beta C}$, we obtain

$$W_{i,i+1} = P e^{-\beta[(\gamma-1)V_i + \gamma V_{i+1} + (1-\eta)(U_{i+1} - U_i)]}. \quad (8)$$

Let us compare this with Eq. (5). Since the values of U_i and U_{i+1} are, in principle, arbitrary, we have that $\alpha - 1 = -1 + \eta$ and $\alpha = 1 - \eta$ and therefore $\alpha = \eta = 1/2$. This result is actually a consequence of the inversion symmetry assumed in (4). Finally, the expression for the transition probability is

$$W_{i,i+1} = P e^{-\beta[(\gamma-1)V_i + \gamma V_{i+1} + \Delta U/2]}, \quad (9)$$

with $\Delta U = U_{i+1} - U_i$.

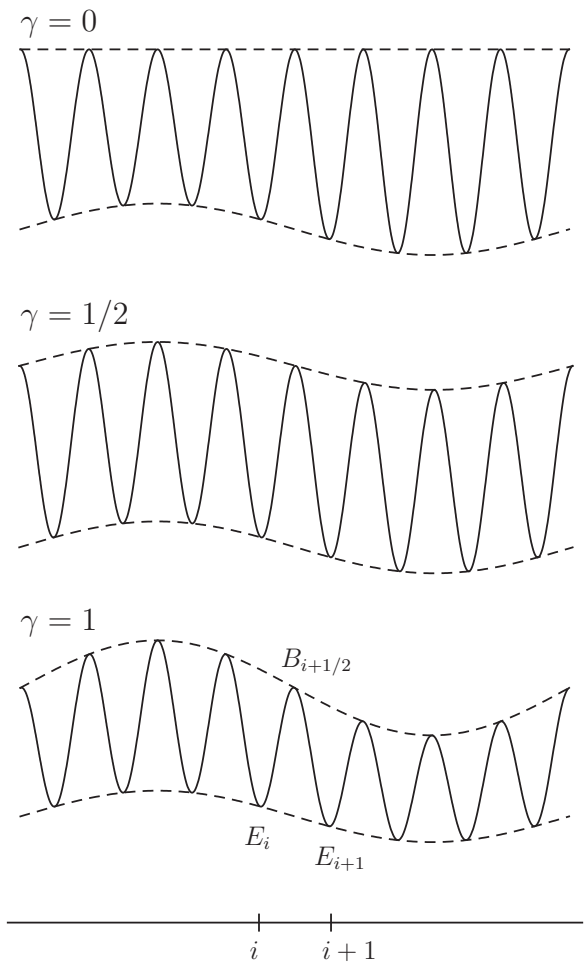

FIG. 1. Energy landscape of wells E_i and barriers $B_{i+1/2}$. From top to bottom $\gamma = 0$, $1/2$, and 1 $\forall i$. In this illustration, C is constant and $U_i = 0 \forall i$.

The previous arguments allow us to construct an energy landscape that gives physical meaning to the parameters and variables involved in the transition probability. In this picture we are using the Hänggi interpretation [27] of the Langevin equation with multiplicative noise, or the barrier model [28], for which the particle current, without external potential and in a continuous space, is $J = -D(x)\frac{\partial n}{\partial x}$ (for other interpretations, the spatial dependent diffusion coefficient is inside the space derivative [28]).

In principle, γ can take any real value. We conjecture that, from a physical point of view, the pertinent values of γ are in the range $[0,1]$. Typical situations are shown in Fig. 1. For $\gamma = 0$, the transition probability depends on the origin potential

$$W_{i,i+1} = P e^{-\beta(-V_i + \Delta U/2)} \quad (\gamma = 0). \quad (10)$$

For $\gamma = 1$, the transition depends on the target potential

$$W_{i,i+1} = P e^{-\beta(V_{i+1} + \Delta U/2)} \quad (\gamma = 1). \quad (11)$$

For $\gamma = 1/2$ we have an intermediate case that is a frequent choice in Monte Carlo (MC) simulations of diffusion processes; the transition depends on the energy difference between target and origin potentials

$$W_{i,i+1} = Pe^{-\beta(\Delta V+\Delta U)/2} \quad (\gamma = 1/2), \tag{12}$$

with $\Delta V = V_{i+1} - V_i$.

III. CURRENT AND FOKKER-PLANCK EQUATION

The current J between sites i and $i+1$ is

$$J = n_i W_{i,i+1} - n_{i+1} W_{i+1,i}. \tag{13}$$

We substitute (9) in (13). Now we turn to a continuous description in which n_i is replaced by $n(x)$, V_i by $V(n(x))$, and U_i by $U(x)$, with $x = ai$; we approximate $(n_{i+1} - n_i)/a \simeq \frac{\partial n}{\partial x}$, $(V_{i+1} - V_i)/a \simeq \frac{dV}{dn}\frac{\partial n}{\partial x}$, and $(U_{i+1} - U_i)/a \simeq \frac{\partial U}{\partial x}$. We call $D_0 = Pa^2$ the free-diffusion coefficient. After some algebra, we obtain (more details are in the Appendix)

$$Ja = -\mu \frac{\partial U}{\partial x} n - D\frac{\partial n}{\partial x}, \tag{14}$$

where the mobility μ and the diffusion coefficient D are

$$\mu = \beta D_0 e^{-\beta(2\gamma-1)V}, \tag{15}$$

$$D = D_0 e^{-\beta(2\gamma-1)V}\left(\beta n \frac{dV}{dn} + 1\right). \tag{16}$$

In the previous derivation the validity of the Ginzburg criterion for a mean-field theory is assumed: The fluctuations are small enough so that $(\langle n_i^2\rangle - \langle n_i\rangle^2)/\langle n_i^2\rangle \ll 1$. The relation between the mobility and diffusion coefficient

$$D = \mu\beta^{-1}\left(\beta n \frac{dV}{dn} + 1\right) \tag{17}$$

does not depend on γ. In the absence of an interaction, we recover the Einstein relation $D = \mu\beta^{-1}$.

The resulting Fokker-Planck equation

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(\mu \frac{\partial U}{\partial x} n + D\frac{\partial n}{\partial x}\right) \tag{18}$$

is nonlinear because of the dependence of μ and D on n and $V(n)$. It is a free-energy Fokker-Planck equation with Boltzmann statistics (see Chap. 5 in [2]). If we consider the notation used in Eq. (5.4) of Ref. [2], we find the following correspondence: $n \to P$, $\beta U \to U_0/Q$, $\beta V \to \frac{\delta U_{\rm NL}}{\delta P}/Q$, and $D_0 \to Q$. The main difference of our approach is the introduction of the parameter γ, which plays a relevant role in the system's dynamics, and its physical interpretation in the energy landscape.

Identifying the zero-current state with equilibrium, it is easy to see that the equilibrium concentration is $n_{\rm eq} \propto e^{-\beta(V+U)}$. The proportionality constant can be written as

$$n_{\rm eq} = e^{-\beta(V+U-\mu_c)}, \tag{19}$$

where we can identify μ_c with the chemical potential. As expected, γ plays no role in the equilibrium solution. Its influence is present in the dynamics through the dependence of μ and D on γ. Let us also note that the parameter γ has influence only when an interaction potential is present.

IV. MEAN-FIELD POTENTIAL

Instead of speaking about the energy of one particle, as in (1), let us consider the energy of the configuration of n_i particles

$$\epsilon_i = \Phi(n_i) + n_i U_i, \tag{20}$$

where $\Phi(n_i)$ is the interaction energy of the configuration of n_i particles. The question that lies at the core of a mean-field theory is what the relation is between V and Φ.

In order to answer this question we have to appeal to the microscopic description given by the grand partition function for classical particles. Since there is no interaction between different lattice sites, it can be written as

$$\Xi = \prod_i Z_i, \tag{21}$$

with

$$Z_i = \sum_{n_i=0}^{\infty} \frac{1}{n_i!} e^{-\beta(\epsilon_i - n_i\mu_c)} = \sum_{n_i=0}^{\infty} \frac{1}{n_i!} e^{-\delta_i n_i - \beta\Phi(n_i)}, \tag{22}$$

where, for simplicity, we introduced $\delta_i = \beta(U_i - \mu_c)$. We can obtain the equilibrium mean value $\langle n_i\rangle$ with

$$\langle n_i\rangle = -\frac{\partial \ln Z_i}{\partial \delta_i} \tag{23}$$

and express this result as a function of δ_i (for a given value of β): $\langle n_i\rangle = f_\beta(\delta_i)$. This means that we can consider δ_i as a parameter that allows us to scan the possible values of $\langle n_i\rangle$. From an experimentalist point of view, we can apply a varying external potential and measure the possible values of $\langle n_i\rangle$. We will restrict ourself to situations in which f_β is invertible, i.e., we can write $\delta_i = f_\beta^{-1}(\langle n_i\rangle)$; this precludes the possibility of phase transitions, for which, for a given δ_i, there could be more than one value of $\langle n_i\rangle$.

The connection with the description of the previous section, based on the nonlinear Fokker-Planck equation, is given by the fact that $\langle n_i\rangle$ should be equal to $n_{\rm eq}$ in $x = ai$. Then, using (19), we have

$$\langle n_i\rangle = e^{-\beta V - \delta_i}. \tag{24}$$

In the same way that we considered that the transition probabilities satisfy the detailed balance relation even when the system is out of equilibrium, we can consider that the relation between the mean-field potential V and the particle concentration that we can derive from the previous equation also holds out of equilibrium. This can be justified using the local equilibrium assumption. For simplicity, we replace $\langle n_i\rangle$ by n. Therefore, from (24) we obtain

$$V(n) = -\beta^{-1}\left[\ln n + f_\beta^{-1}(n)\right]. \tag{25}$$

The most simple situation is zero interaction; in this case $n = e^{-\delta_i}$ and $f_\beta^{-1}(n) = -\ln n$. A more direct relation between V and Φ can be derived from (24); it also clarifies its physical

meaning. We have

$$
\begin{aligned}
e^{-\beta V} &= -e^{\delta_i}\frac{\partial \ln Z_i}{\partial \delta_i} = \frac{e^{\delta_i}}{Z_i}\sum_{n_i=0}^{\infty}\frac{n_i}{n_i!}e^{-\delta_i n_i-\beta\Phi(n_i)} \\
&= \frac{1}{Z_i}\sum_{n_i=1}^{\infty}\frac{1}{(n_i-1)!}e^{-\delta_i(n_i-1)-\beta\Phi(n_i)} \\
&= \frac{1}{Z_i}\sum_{n_i'=0}^{\infty}\frac{1}{n_i'!}e^{-\delta_i n_i'-\beta\Phi(n_i'+1)} \\
&= \frac{1}{Z_i}\sum_{n_i'=0}^{\infty}e^{-\beta[\Phi(n_i'+1)-\Phi(n_i')]}\frac{1}{n_i'!}e^{-\delta_i n_i'-\beta\Phi(n_i')} \\
&= \langle e^{-\beta[\Phi(n_i+1)-\Phi(n_i)]}\rangle. \qquad (26)
\end{aligned}
$$

We can interpret this result using the Jarzynski equality [29], also called the Bochkov-Kuzovlev-Jarzynski equality [30]. It gives a relation between the Helmholtz free-energy variation ΔF and the applied work W:

$$e^{-\beta\Delta F} = \langle e^{-\beta W}\rangle. \qquad (27)$$

Comparing (26) and (27), we can see that the mean-field potential V at a given point is equal to the free-energy change when the work needed to increase the number of particles by one, $W = \Phi(n_i+1) - \Phi(n_i)$, is applied to that point.

V. FERMIONS

Hard-core interaction is the prototypical case study. As mentioned in the Introduction, an interaction that becomes infinite for particles occupying the same state is analogous to the Pauli exclusion principle for fermions. Phenomenological arguments to determine the transition probabilities are usually presented [3,22,25,31]. In the absence of an external field, the transition probability from i to $i+1$ is proportional to the quantity $1-n_{i+1}$, which indicates if the target site is free to be occupied by the incoming particle:

$$W_{i,i+1} = P(1-n_{i+1}). \qquad (28)$$

Since the transition probability depends on the target site, we have $\gamma = 1$. From Eq. (11) we obtain $V_{i+1} = -\beta^{-1}\ln(1-n_{i+1})$. In the continuous limit and neglecting fluctuations,

$$V(n) = -\beta^{-1}\ln(1-n). \qquad (29)$$

Once the mean-field potential is obtained this way, we can turn to the more general situation in which an external potential U is present. The resulting equilibrium concentration, which is obtained by substituting (29) in (19), corresponds to Fermi-Dirac statistics: $n_{\rm eq} = 1/(e^{\beta(U-\mu_c)}+1)$. Let us emphasize that these results hold only for collective diffusion of indistinguishable particles, i.e., this mean-field approach does not hold for diffusion of tagged particles.

On the other hand, using the interaction energy

$$\Phi(n_i) = \begin{cases} 0 & \text{for} \quad n_i = 0,1 \\ \infty & \text{for} \quad n_i \geqslant 2 \end{cases} \qquad (30)$$

in (26), we can arrive at the same result (29). This procedure does not appeal to an *a priori* definition of the transition probabilities with the shape of (28) and makes a clear distinction between the mean-field potential V and the microscopic interaction energy Φ.

Several results obtained from diffusion in a lattice indicate that the hard-core interaction does not have any effect on the collective diffusion coefficient [3,5,22,25]

$$D_{\rm HC} = D_0, \qquad (31)$$

a relation that holds in the limit of zero size particles. (Of course, the interaction *does* have an effect on the single-particle diffusion coefficient [32,33].) This result is obtained from the expression for the diffusion coefficient (16) using (29) for the mean-field potential and $\gamma = 1$.

Therefore, in our description based on the γ-dependent energy landscape, the result (31) corresponds to a constant value of γ equal to 1. However, this is not the only possibility. For example, for $\gamma = 1/2$ and the same hard-core interaction we obtain

$$D_{\rm HC} = \frac{D_0}{1-n} \quad (\gamma = 1/2). \qquad (32)$$

It is interesting to note that a similar dependence of the diffusion coefficient on the concentration has been obtained for hard spheres in a continuous space (see, for example, [8,12,13,23]). More complex expressions of the diffusion coefficient can be obtained if the parameter γ that depends on the concentration is considered. In all cases the equilibrium solution is the same.

Now we consider the situation in which multiple occupancy is allowed with a maximum number of particles N. Let us call m_i the number of particles at site i to distinguish this case from the one of the preceding paragraphs. Let us consider that the average concentration is given by $\langle m_i\rangle = N\langle n_i\rangle$. In terms of the partition function,

$$\langle m_i\rangle = -N\frac{\partial \ln Z_i}{\partial \delta_i} = -\frac{\partial \ln Z_i^N}{\partial \delta_i}. \qquad (33)$$

Then the partition function for the multiple occupancy case is

$$Z_i' = (1+e^{-\delta_i})^N = \sum_{m_i=0}^{N} e^{-\delta_i m_i}\binom{N}{m_i}. \qquad (34)$$

Using the definition of the partition function and comparing with the previous equation, we obtain the interaction energy for this case:

$$\Phi'(m_i) = \begin{cases} -\beta^{-1}\ln\frac{N!}{(N-m_i)!} & \text{for} \quad 0 \leqslant m_i \leqslant N \\ \infty & \text{for} \quad m_i > N. \end{cases} \qquad (35)$$

The mean-field potential is

$$V(m) = -\beta^{-1}\ln(N-m). \qquad (36)$$

By increasing the value of N we increase the mean number of particles at each site and reduce fluctuations, a procedure that favors the conditions for the validity of the Fokker-Planck equation. Equation (36) is a generalization of the mean-field potential for multiple occupancy; Eq. (29) is recovered for $N = 1$. Using (36) in (9), the transition probability is

$$W_{i,i+1} = P(N-m_i)^{\gamma-1}(N-m_{i+1})^{\gamma}e^{-\beta\Delta U/2}.$$

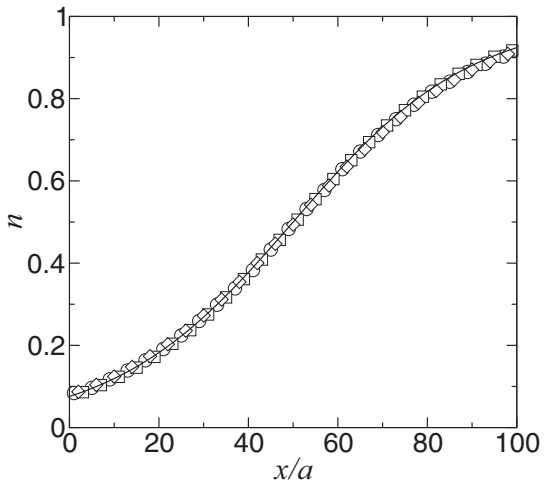

FIG. 2. Equilibrium concentration n for classical fermions with $U(x) = -Fx$, $\beta Fa = 0.05$, and total concentration 0.5. The curve corresponds to the Fermi-Dirac distribution and the dots to Monte Carlo simulations with different values of γ: $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). The same distribution is attained for all values of γ. Simulations were made with multiple occupancy of sites, $n_i = m_i/N$. The following are the other parameters: number of samples, 1000; MC steps for each sample, 10^7 ($\gamma = 0,1$ and $N = 100$) or 10^8 ($\gamma = 1/2$ and $N = 500$); fixed boundary conditions; and system size, $L = 100a$.

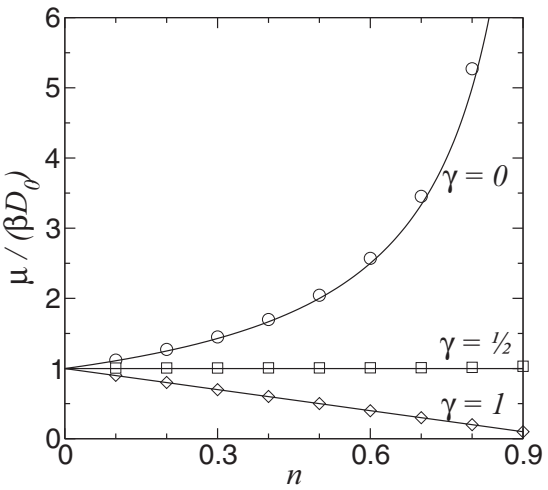

FIG. 3. Fermion's mobility μ against concentration n for different values of γ, obtained from a system with homogeneous concentration, constant force $\beta Fa = 0.05$, and periodic boundary conditions (see the text for more details). The curves correspond to Eq. (15). Dots correspond to Monte Carlo simulations with $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). The following are the other parameters: number of samples, 1000; MC steps, between 10^5 and 10^6; $N = 100$; and system size, $L = 100a$.

This could have divergences for $\gamma < 1$. For $\gamma < 1$ it is necessary to consider multiple occupancy and N large enough in order to have $m_i < N$ for all sites. Instead of a hard-core interaction we have a repulsive soft-core interaction that generates the same Fermi-Dirac distribution in equilibrium (Fig. 2).

For example, for $\gamma = 1/2$, the transition probability is

$$W_{i,i+1} = P\sqrt{\frac{N - m_{i+1}}{N - m_i}}e^{-\beta\Delta U/2} \quad (\gamma = 1/2),$$

which depends on the origin and target sites. Then, in the hopping model for $\gamma = 1/2$, particles tend to jump with a larger probability when they come from a site with many particles and when they go to a site with few particles.

Figure 2 shows the equilibrium solution with a constant force to the right in a closed system and Monte Carlo simulation results for different values of γ (0, 1/2, and 1); as expected, in all cases the same equilibrium solution is obtained. As mentioned before, the different values of γ become relevant in nonequilibrium situations. We analyzed two simple cases. The first one is a constant force ($U = -Fx$) applied to a system with periodic boundary conditions. The nonequilibrium stationary state is homogeneous with nonzero current. From Eq. (14) we can obtain the mobility $\mu = Ja/nF$. Figure 3 shows numerical simulation results of the mobility against concentration for different values of γ. The results coincide with the analytical curve (15). The analytical expressions of μ and D, for fermions and bosons (in the next section) and for different values of γ, are shown in Table I.

The second nonequilibrium situation that we consider is zero force with unequal fixed boundary conditions. The difference in particle concentration at both ends of the system produces a constant current in the stationary state. Numerically, we can obtain the density profile and also its space derivative. From the equation for the current (14), we have that the diffusion coefficient is $D = -Ja/\frac{\partial n}{\partial x}$. In this way, we can plot the diffusion coefficient against concentration for different values of γ, as shown in Fig. 4. The numerical results again coincide with the analytical results (16) (see Table I).

VI. BOSONS

Boson statistics can be obtained in a classical context using a statistical potential. The behavior of quantum noninteracting particles can be reproduced by classical particles with this effective attractive interaction, which is given by

$$\Phi(n_i) = -\beta^{-1} \ln n_i! \tag{37}$$

Its effect is to cancel the Gibbs factor in the partition function (22), from which the Bose-Einstein distribution is obtained.

TABLE I. Mobility and diffusion coefficient as derived from Eqs. (15) and (16), for fermions (minus sign) and bosons (plus sign). The general expressions as functions of γ are shown in the first row and the expressions for the values of γ used in the figures are in the subsequent rows.

γ	$\mu/D_0\beta$	D/D_0
γ	$(1 \pm n)^{2\gamma-1}$	$(1 \pm n)^{2\gamma-2}$
$\gamma = 0$	$1/(1 \pm n)$	$1/(1 \pm n)^2$
$\gamma = 1/2$	1	$1/(1 \pm n)$
$\gamma = 1$	$1 \pm n$	1

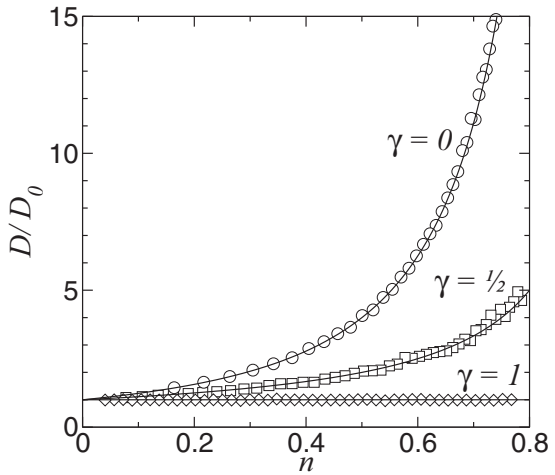

FIG. 4. Fermion's diffusion coefficient D against concentration n for different values of γ, obtained from a system with unequal fixed conditions at the ends and zero force, in a nonequilibrium stationary state (constant current J; see the text for more details). The curves correspond to Eq. (16). Dots correspond to Monte Carlo simulations with $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). The following are the other parameters: number of samples, 1000; MC steps, between 10^8 and 10^9; $N = 500$; system size, $L = 100a$; $n(0) = 0.8$; and $n(L) = 0$.

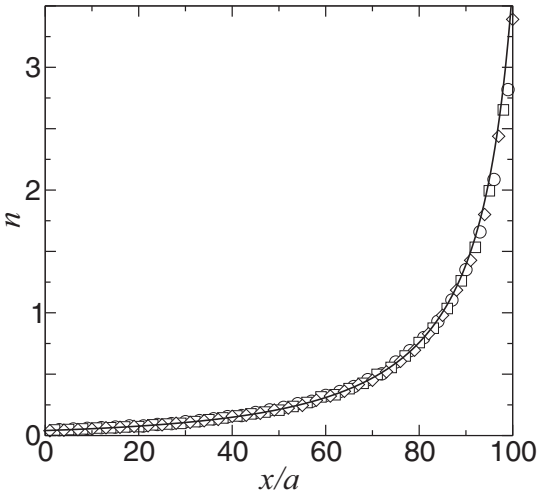

FIG. 5. Equilibrium concentration n for bosons with energy $U(x) = -Fx$, $\beta Fa = 0.03$, and total concentration 0.5. The curve corresponds to the Bose-Einstein distribution and the dots to Monte Carlo simulations with different values of γ: $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). In order to reduce simulation fluctuations, we define the concentration n_i at site i as $n_i = m_i/N$, where m_i is the number of particles in this site. The following are the other parameters: number of samples, 1000; MC steps for each sample, 10^7; $N = 10$; fixed boundary conditions; and system size, $L = 100a$.

It is not difficult to obtain the corresponding mean-field potential from (26):

$$V(n) = -\beta^{-1}\ln(1+n). \tag{38}$$

The equilibrium Bose-Einstein distribution is recovered when this result is substituted in (19): $n_{\rm eq} = 1/(e^{\beta(U-\mu_c)} - 1)$. Figure 5 shows this equilibrium solution with a constant force to the right. The figure also presents numerical results for different values of γ, showing that in all cases the same solution is attained.

The same procedure used in the previous section to extend the mean-field potential of hard-core interaction to the multiple occupancy case can also be applied for bosons. The motivation in this case is to reduce fluctuations. Considering that $m_i = Nn_i$, the mean-field potential in terms of m in the continuous limit is

$$V(m) = -\beta^{-1}\ln(N+m). \tag{39}$$

The expression reduces to (38) when $N = 1$. Substituting in (9), the transition probability is

$$W_{i,i+1} = P(N+m_i)^{\gamma-1}(N+m_{i+1})^{\gamma}e^{-\beta\Delta U/2}.$$

For example, for $\gamma = 1/2$ we have

$$W_{i,i+1} = P\sqrt{\frac{N+m_{i+1}}{N+m_i}}e^{-\beta\Delta U/2} \quad (\gamma = 1/2).$$

The interaction is attractive. The transition probability becomes larger when the origin site has few particles and when the target site has many particles.

As in the case of hard-core interaction (or fermions), the mean-field potential determines the equilibrium solution but not the dynamics. The mobility and diffusion coefficient are not unequivocally determined by V; they depend also on γ. As in the previous section, we analyzed two nonequilibrium steady-state situations from which the mobility and the diffusion coefficient against concentration can be obtained. Numerical results coincide with the corresponding equations (15) and (16), as shown in Figs. 6 and 7. In all cases, for fermions or bosons, in the limit of low concentration, both the mobility and the diffusion coefficient coincide with the corresponding noninteracting values βD_0 and D_0 respectively.

VII. GENERALIZATIONS

The generalization of the nonlinear Fokker-Planck equation (18) to higher dimensions is straightforward:

$$\frac{\partial n}{\partial t} = \nabla\cdot(\mu\nabla U n + D\nabla n). \tag{40}$$

The expressions (15) and (16) for μ and D remain unchanged. The relation (26) between V and Φ also keeps its validity for higher dimensions. Let us note that these equations also hold for a space-dependent parameter γ.

For the generalization to continuous systems we have to take into account some considerations. The system is divided into cells of size a, small enough to be considered pointlike and, at the same time, large enough to contain many particles (a standard approach in nonequilibrium statistical mechanics). The cell size is much smaller than a typical concentration wave number λ. Also, the interaction range r should be much smaller than the cell size. So we have $r \ll a \ll \lambda$.

The condition $a \ll \lambda$ allows us to take the continuous limit and obtain the Fokker-Planck equation. The condition $r \ll a$ allows us to neglect the interaction between cells, since the

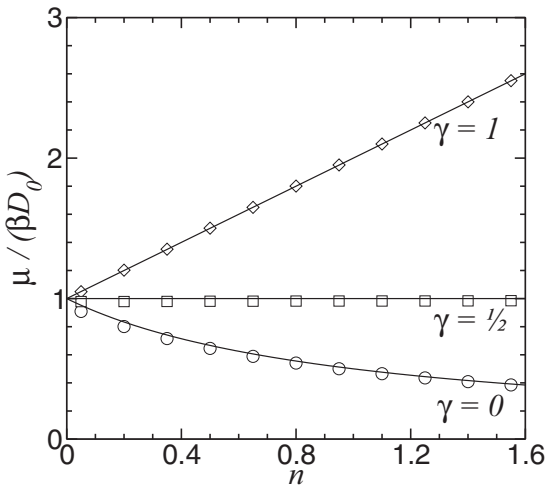

FIG. 6. Boson's mobility μ against concentration n for different values of γ, obtained from a system with homogeneous concentration, constant force $\beta Fa = 0.05$, and periodic boundary conditions. The curves correspond to Eq. (15). Dots correspond to Monte Carlo simulations with $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). The following are the other parameters: number of samples, 5000; MC steps, between 10^5 and 6×10^6; $N = 20$; system size, $L = 100a$.

interaction energy in the cell's surface is much smaller than in the bulk, and to keep the validity of the relation (26) between V and Φ. The consequence is that the Fokker-Planck equation is local. In this case, the parameter γ is associated with an *effective* energy landscape, in the same sense that $V(n)$ is an effective potential.

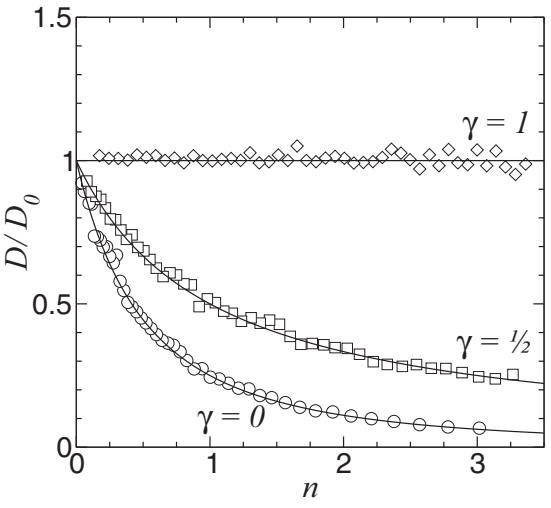

FIG. 7. Boson's diffusion coefficient D against concentration n for different values of γ, obtained from a system with unequal fixed conditions at the ends and zero force, in a nonequilibrium stationary state. The curves correspond to Eq. (16). Dots correspond to Monte Carlo simulations with $\gamma = 0$ (circles), $\gamma = 1/2$ (squares), and $\gamma = 1$ (diamonds). The following are the other parameters: number of samples, 5000; MC steps, between 10^7 and 10^8; $N = 100$; system size, $L = 100a$; $n(0) = 3.5$, and $n(L) = 0$.

VIII. EXPERIMENTAL TEST

Taking advantage of the generalization to a continuous system mentioned in the previous section, we can propose experiments of diffusion of a solute in, for example, water, to validate part of the results. The concentration range of the solute should be large enough in order to reach values for which the interaction among particles becomes relevant.

The experimental setup for the measurement of the mobility and diffusion coefficient may be based on the situations described in Sec. V. The mobility can be obtained from a system with constant force and equal fixed concentration at both ends; it has a homogeneous concentration in the nonequilibrium steady state. The diffusion coefficient can be obtained from the steady-state current and concentration gradient of a system without force, but with unequal fixed concentrations at the ends.

Let us suppose that the mobility and diffusion coefficient are measured as functions of the concentration, $\mu(n)$ and $D(n)$, and that for large enough values of n they depart from their free-diffusion values (βD_0 and D_0, respectively). The specific shape of these functions depends on the details of the interactions among the substances chosen for the experiment. Nevertheless, we can expect that, for example, for a repulsive interaction, the diffusion coefficient would increase as n increases, as qualitatively shown in Fig. 4. The concentration per site n is related to the concentration per unit length by $c = n/a$. If, for a repulsive interaction, $c_{\max}$ is the maximum possible value of c, we have $n = c/c_{\max}$.

From (17) we obtain an equation for $V(n)$,

$$\frac{dV}{dn} = \frac{1}{\beta n}\left(\frac{\beta D(n)}{\mu(n)} - 1\right), \tag{41}$$

that can be solved with the condition $V(0) = 0$. With $V(n)$ we can obtain γ from (15)

$$\gamma = \frac{1}{2}\left(1 - \frac{1}{\beta V(n)} \ln \frac{\mu(n)}{\beta D_0}\right). \tag{42}$$

In the examples of Secs. V and VI, we assumed constant values of γ for simplicity. We can see in Eq. (42) that, in general, γ is a function of n. Therefore, measurements of $\mu(n)$ and $D(n)$ can be used to experimentally check, for example, our conjecture that γ remains bounded between 0 and 1.

IX. CONCLUSION

We derived a nonlinear Fokker-Planck equation for interacting particles. The derivation is based on an energy landscape of wells and barriers on a lattice. The mean-field potential and the external potential determine the energy wells and the equilibrium solution. The barrier's heights depend on the parameter γ; it determines if the transition probability depends on the mean-field potential of the origin site, the target site, or on a mixture of both.

A relation between the mean-field potential and the microscopic interaction energy was deduced. The Jarzynski equality can be used to interpret the mean-field potential as the free-energy change when the work needed to increase the number of particles by one is applied.

The results are illustrated with the hard-core (or fermion) and boson interactions. The corresponding mean-field potentials can be combined with different values of γ. The consequence is that, for the same potential and equilibrium solution, the dependence of the mobility and diffusion coefficient on the concentration can have large variations determined by the value of γ. In all cases, for small concentration, the mobility and diffusion coefficient tend to the corresponding noninteracting values.

We considered only different constant values of γ but, in general, it could be a function of the position or of the concentration. Measurements of the mobility and the diffusion coefficient as functions of the concentration can be used to obtain experimental values of γ.

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APPENDIX

We present here a more detailed derivation of Eqs. (14)–(16). Using the expression for the transition probabilities (9) in (13) we have

$$J = n_i P e^{-\beta[(\gamma-1)V_i+\gamma V_{i+1}+\Delta U/2]} - n_{i+1} P e^{-\beta[(\gamma-1)V_{i+1}+\gamma V_i-\Delta U/2]}.$$

In the continuous limit we approximate $V_{i+1} \simeq V + \frac{dV}{dn}\frac{\partial n}{\partial x}a$, $n_{i+1} \simeq n + \frac{\partial n}{\partial x}a$, and $\Delta U \simeq \frac{\partial U}{\partial x}a$. Substituting in the expression for the current, we have

$$J = Pe^{-\beta(2\gamma-1)V}\left\{n\exp\left[-\beta a\left(\gamma\frac{dV}{dn}\frac{\partial n}{\partial x}+\frac{1}{2}\frac{\partial U}{\partial x}\right)\right] - \left(n+\frac{\partial n}{\partial x}a\right)\exp\left[-\beta a\left((\gamma-1)\frac{dV}{dn}\frac{\partial n}{\partial x}-\frac{1}{2}\frac{\partial U}{\partial x}\right)\right]\right\}.$$

The Ginzburg criterion was used to decorrelate products of nonlinear terms. We expand the exponentials inside the curly brackets and keep terms up to order a:

$$\begin{aligned} J &= Pe^{-\beta(2\gamma-1)V}\left\{n\left[1-\beta a\left(\gamma\frac{dV}{dn}\frac{\partial n}{\partial x}+\frac{1}{2}\frac{\partial U}{\partial x}\right)\right] - \left(n+\frac{\partial n}{\partial x}a\right)\left[1-\beta a\left((\gamma-1)\frac{dV}{dn}\frac{\partial n}{\partial x}-\frac{1}{2}\frac{\partial U}{\partial x}\right)\right]\right\} \\ &= -Pae^{-\beta(2\gamma-1)V}\left\{n\beta\frac{\partial U}{\partial x}+\left(\beta n\frac{dV}{dn}+1\right)\frac{\partial n}{\partial x}\right\}. \end{aligned}$$

We can identify the mobility as the factor that multiplies the external potential gradient times n and the diffusion coefficient as the one that multiplies the concentration gradient:

$$Ja = -\underbrace{\beta D_0 e^{-\beta(2\gamma-1)V}}_{\mu} n\frac{\partial U}{\partial x} - \underbrace{D_0 e^{-\beta(2\gamma-1)V}\left(\beta n\frac{dV}{dn}+1\right)}_{D}\frac{\partial n}{\partial x},$$

where we have replaced Pa^2 by D_0. The factor a that appears on the left-hand side is canceled when, instead of the particle number per site, we consider the concentration per unit length $c = n/a$.

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