Correlation corrections to the conductivity of one-dimensional disordered hopping models

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Transport on a one-dimensional nonuniform periodic chain with a hard-core interaction is examined. The mean-field conductivity is rederived, and the first correction due to many-particle effects is obtained. By letting the period go to infinity, the results are extended to nonperiodic chains, including the random one. The case of the site-disordered system with two values of the site energy is discussed in detail.

I. INTRODUCTION

Of the many interesting aspects of hopping transport, two have polarized the attention of many theoreticians during the past two decades.

First, there is the problem of transport through disordered lattices, with particular emphasis on one-dimensional systems (a review of the results up to 1981 is given in the paper of Alexander *et al.*[1]). Exact formulas for the velocity and the diffusion coefficient were obtained by Derrida.[2] This subject has been studied intensively[3,4] (see also the references cited in Ref. 4). The problem treated by these papers was essentially the random walk (of one particle) in a random environment.

Second, there is correlated hopping. The interactions among particles diffusing on a lattice may be treated in the mean-field (MF) approximation. This leads to a one-particle description, which often proves to be far from accurate for real systems. In many cases, one has to take into account dynamic correlations due to the interactions. The simplest interaction, namely, the hard-core one, which prevents the double occupation of one site, makes correlations important in the case of tracer diffusion[5,6] and in the case of collective (chemical) diffusion.[5,7] The influence of correlations caused by more complex interactions has also been studied (see Ref. 8 and the references cited therein). All these papers dealt with correlated hopping on periodic structures.

To our knowledge, the only paper to date intermediate between these two trends was that of Tahir-Kheli[9] which dealt with the effects of disorder on the correlated tracer diffusion in one dimension.

In the present paper, we present a calculation of the hopping conductivity of a disordered one-dimensional lattice by taking correlations into account. We deal only with the hard-core repulsion among particles diffusing on a nonuniform chain.

In Sec. II, we obtain a formula that gives the first correction to the MF result for the conductivity of particles hopping on a periodic one-dimensional lattice with an arbitrary length of the elementary cell. This is done by a stationary-flow approach due to Richards,[5] which was also used in earlier papers.[8,10] By letting the period

go to infinity, the results are extended to nonperiodic chains. The first nontrivial correction is obtained by keeping the nearest-neighbor dynamic correlator and neglecting all the others.

In Sec. III we consider the particular case of a chain with only two values for the site energies. A comparison is made between one exactly soluble model, some other periodic models, and the disordered one.

Some conclusions are drawn in Sec. IV.

II. THE CORRELATION FACTOR

A. The model

We consider a periodic one-dimensional lattice with N equidistant sites per elementary cell and N_c cells. Site i has energy ε_i. There are N_p particles with electric charge e in the system and the concentration is given by

$$c = \frac{N_p}{NN_c} . \tag{2.1}$$

An infinite chain is obtained by taking replicas of this system and by imposing Born–von Kármán cyclic conditions for all the site-dependent quantities.

The occupation number of site i is denoted by n_i and it takes the values 0 and 1 for an empty and an occupied site, respectively. The concentration c may assume any value in the interval $[0,1]$.

A particle on site i may jump to one of the two nearest-neighbor (NN) sites $i \pm 1$, only if the final site is empty (Fig. 1), with probability per unit time (or jump rate) $W_{i,i\pm 1}$. By periodicity, we have
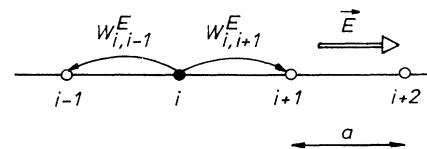

FIG. 1. The hop of a particle to a NN vacant site. The direction of the electric field is indicated.

$$\varepsilon_{i+N} = \varepsilon_i, \quad i \in \mathbb{Z} , \tag{2.2}$$

$$W_{i+N, i+N\pm1} = W_{i,i\pm1}, \quad i \in \mathbb{Z} . \tag{2.3}$$

Evolution towards equilibrium is ensured by the detailed-balance condition[5,11]

$$W_{i,i\pm1} f_i (1 - f_{i\pm1}) = W_{i\pm1,i} f_{i\pm1} (1 - f_i) , \tag{2.4}$$

where f_i is the Fermi function given by

$$f_i = \langle n_i \rangle_0 = \{1 + \exp[\beta(\varepsilon_i - \mu)]\}^{-1} \tag{2.5}$$

with $\beta = (kT)^{-1}$ and μ is the chemical potential. The subscript 0 indicates the usual equilibrium average, which is calculated for the hard-core interaction in the same manner as for the free-fermion gas.

We consider a uniform constant electric field E parallel to the chain (Fig. 1). This modifies the jump rate symmetrically as follows:[5,8]

$$W^E_{i,i\pm1} = W_{i,i\pm1} \left[1 \pm \frac{eEa}{2kT} \right] \equiv W_{i,i\pm1}(1\pm\Delta) , \tag{2.6}$$

where a is the NN distance and Δ is a shorthand notation for $eEa/2kT$. Equation (2.6) is suitably chosen to preserve detailed balance up to first order in E, which is enough for the linear response σ, the conductivity. We will systematically discard higher-order terms in Δ. When the steady state is established, σ is given by Ohm's law:

$$\sigma = \frac{j}{E} , \tag{2.7}$$

where j is the current density,

$$j = N_p ev / V = \frac{cev}{a} , \tag{2.8}$$

with v the mean velocity of particles and $V = NN_c a$ is the "volume" of the system. The velocity is proportional to the difference between the mean number of jumps to the right and of those to the left in unit time[5,8] (see also Ref. 12):

$$v = a N_p^{-1} N_c \sum_{i=1}^{N} [W_{i,i+1}(1+\Delta)\langle n_i(1-n_{i+1})\rangle$$
$$- W_{i+1,i}(1-\Delta)\langle n_{i+1}(1-n_i)\rangle]$$
$$\equiv a N_p^{-1} N_c \sum_{i=1}^{N} \xi_i . \tag{2.9}$$

In Eq. (2.9) the $\langle \ \rangle$ brackets indicate steady-state averages. No systematic way is known for calculating these quantities, but they have one useful property which was used in writing Eq. (2.9): They are invariant under translation with aN. We also introduced the shorthand notation ξ_i for the whole quantity in the square brackets on the right-hand side of Eq. (2.9).

In order to evaluate the velocity, we write down the rate equation for the evolution of the time-dependent mean occupation number of site i:[5,11]

$$\frac{d\langle n_i \rangle_t}{dt} = -\xi_i(t) + \xi_{i+1}(t) . \tag{2.10}$$

Let δ_i be the deviation of n_i from its equilibrium value f_i:

$$n_i = f_i + \delta_i . \tag{2.11}$$

Let us write ξ_i in terms of δ_i:

$$\xi_i = W_{i,i+1}(1+\Delta)[f_i(1-f_{i+1}) + (1-f_{i+1})\langle \delta_i \rangle - f_i \langle \delta_{i+1} \rangle - \langle \delta_i \delta_{i+1} \rangle]$$
$$- W_{i+1,i}(1-\Delta)[f_{i+1}(1-f_i) + (1-f_i)\langle \delta_{i+1} \rangle - f_{i+1} \langle \delta_i \rangle - \langle \delta_i \delta_{i+1} \rangle] . \tag{2.12}$$

Equation (2.12) is much simplified by introducing the following "symmetrized" jump rates:

$$\mathcal{W}_{i,i+1} \equiv w_{i,i+1} f_i(1-f_{i+1}) = \mathcal{W}_{i+1,i} \tag{2.13}$$

and a "normalized" deviation η_i,

$$\eta_i = \frac{\delta_i}{a_i} \frac{n_i - f_i}{a_i} , \tag{2.14}$$

where by a_i we have denoted

$$a_i = f_i(1 - f_i) . \tag{2.15}$$

Equation (2.12) is now easily rewritten as

$$\xi_i = \mathcal{W}_{i,i+1}[2\Delta + \langle \eta_i \rangle - \langle \eta_{i+1} \rangle + (f_i - f_{i+1})\langle \eta_i \eta_{i+1} \rangle] , \tag{2.16}$$

where we have used the obvious relation[5,8]

$$\langle \eta_i \rangle = o(\Delta) \tag{2.17}$$

and we have kept only terms of order Δ, as discussed before.

B. The mean-field conductivity

The first approximation is obtained by neglecting all correlations, i.e., by taking

$$\langle \eta_i \eta_{i+1} \rangle = 0 , \tag{2.18}$$

which means considering only linear nonequilibrium effects.

In the absence of the field, this would lead to the following rate equation (see also Ref. 11):

$$\frac{d\langle \eta_i \rangle_t}{dt} = \frac{1}{a_i}[\mathcal{W}_{i,i+1}(\langle \eta_{i+1} \rangle_t - \langle \eta_i \rangle_t)$$
$$+ \mathcal{W}_{i,i-1}(\langle \eta_{i-1} \rangle_t - \langle \eta_i \rangle_t)] , \quad (2.19)$$

which is essentially the one-particle equation, which has been the starting point in studying the random walk in a random medium[1-4] mentioned in our Introduction.

Returning to $E \neq 0$, the steady-state version of Eq. (2.19), or the MF version of Eq. (2.10) in the steady state, reads

$$\mathcal{W}_{i,i+1}(2\Delta + \langle \eta_i \rangle - \langle \eta_{i+1} \rangle)$$
$$= \mathcal{W}_{i,i-1}(2\Delta + \langle \eta_{i-1} \rangle - \langle \eta_i \rangle) , \quad (2.20)$$

which means that both sides of Eq. (2.20) are independent of i. We denote their constant value by C_{MF}:

$$C_{MF} = \mathcal{W}_{i,i+1}(2\Delta + \langle \eta_i \rangle - \langle \eta_{i+1} \rangle) , \quad (2.21)$$

which leads to

$$\langle \eta_{i+1} \rangle = \langle \eta_i \rangle + 2\Delta - C_{MF}\mathcal{W}_{i,i+1}^{-1} \quad (2.22)$$

and finally we get

$$\langle \eta_1 \rangle \equiv \langle \eta_{N+1} \rangle = \langle \eta_1 \rangle + 2N\Delta - C_{MF}\sum_{i=1}^{N}\mathcal{W}_{i,i+1}^{-1} ,$$
$$(2.23)$$

$$C_{MF} = \frac{2\Delta}{\frac{1}{N}\sum_{i=1}^{N}\frac{1}{\mathcal{W}_{i,i+1}}} \equiv 2\Delta\langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1} , \quad (2.24)$$

where by $\langle\langle \cdots \rangle\rangle$ we denote the cell average of a site-dependent quantity.

The MF velocity is now calculated as

$$v_{MF} = aN_p^{-1}N_c\sum_{i=1}^{N}C_{MF} = 2ac^{-1}\Delta\langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1} \quad (2.25)$$

and the MF conductivity is

$$\sigma_{MF} = \frac{j}{E} = \frac{cev_{MF}}{a}\frac{ea}{2kT\Delta} = \frac{e^2 a}{kT}\langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1} .$$
$$(2.26)$$

By the lattice-gas version of the Einstein relation,

$$\sigma = e^2\frac{\partial n}{\partial \mu}D = e^2\frac{\partial}{\partial \mu}\left[\frac{1}{Na}\sum_{i=1}^{N}f_i\right]D$$
$$= \frac{e^2}{akT}\left[\frac{1}{N}\sum_{i=1}^{N}a_i\right]D , \quad (2.27)$$

where $n = N_p/V$, we obtain the MF diffusion coefficient

$$D_{MF} = a^2\frac{\langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1}}{\langle\langle a_i \rangle\rangle} , \quad (2.28)$$

which is proportional to $\langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1}$, a well-known result.[1,2]

It is clear that Eqs. (2.25)–(2.28) are naturally extended to any chain for which the $N \to \infty$ limits of the cell averages exist. One such case is the random chain, where the limit is ensured by the law of large numbers. Of course, other cases (e.g., aperiodic structures) can also be treated in the present scheme.

C. The first-correlation correction

There is one second-order dynamic correlator in the expression of ξ_i, Eq. (2.16), namely, $\langle \eta_i\eta_{i+1} \rangle$. We will take this one into account for all values of i. It involves NN sites and therefore it is the most important of all two-particle correlators (see Ref. 8 for a detailed discussion). Also, as $0 \leq \eta_i \leq 1$, products of more than two η's are smaller and can be neglected. While the accuracy of the approximation cannot be judged by such arguments, they indicate precisely that accounting for $\langle \eta_i\eta_{i+1} \rangle$ represents the first step beyond MF.

Let us introduce the following notation:

$$\lambda_i = (f_{i+1} - f_i)\langle \eta_i\eta_{i+1} \rangle . \quad (2.29)$$

By the same arguments that led to Eq. (2.21) in the MF approximation, we now get, successively,

$$\xi_i = \mathcal{W}_{i,i+1}(2\Delta + \langle \eta_i \rangle - \langle \eta_{i+1} \rangle - \lambda_i) = C , \quad (2.30)$$

$$\langle \eta_{i+1} \rangle = \langle \eta_i \rangle - \lambda_i + 2\Delta - C\mathcal{W}_{i,i+1}^{-1} , \quad (2.31)$$

$$\langle \eta_1 \rangle \equiv \langle \eta_{N+1} \rangle = \langle \eta_1 \rangle + 2N\Delta - C\sum_{i=1}^{N}\mathcal{W}_{i,i+1}^{-1} - \sum_{i=1}^{N}\lambda_i ,$$
$$(2.32)$$

$$C = \langle\langle \mathcal{W}_{i,i+1}^{-1} \rangle\rangle^{-1}\left[2\Delta - \frac{1}{N}\sum_{i=1}^{N}\lambda_i\right]$$
$$= C_{MF}\left[1 - \frac{\langle\langle \lambda_i \rangle\rangle}{2\Delta}\right] . \quad (2.33)$$

The correlation factor of the conductivity is now easily calculated:

$$f = \frac{\sigma}{\sigma_{MF}} = \frac{C}{C_{MF}} = 1 - \frac{\langle\langle \lambda_i \rangle\rangle}{2\Delta} . \quad (2.34)$$

We are left with the evaluation of $\langle\langle \lambda_i \rangle\rangle$. For this purpose we write the rate equation for the evolution of $\langle n_in_{i+1} \rangle_t$. The jumps contributing to its decrease are shown in Fig. 2, while the reverse jumps lead to its increase:
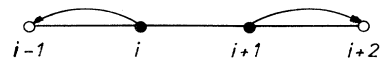

FIG. 2. Jumps that determine the decrease in $\langle n_in_{i+1} \rangle_t$.

$$\frac{d}{dt}\langle n_i n_{i+1}\rangle_t = -f_i \xi_{i+1} + f_{i+1}\xi_i + a_i \mathcal{W}_{i+1,\,i+2}(\langle \eta_i \eta_{i+2}\rangle_t - \langle \eta_i \eta_{i+1}\rangle_t)$$

$$+ a_{i+1}\mathcal{W}_{i-1,\,i}(\langle \eta_{i+1}\eta_{i-1}\rangle_t - \langle \eta_i \eta_{i+1}\rangle_t) + a_i(f_{i+2}-f_{i+1})\mathcal{W}_{i+1,\,i+2}\langle \eta_i \eta_{i+1}\eta_{i+2}\rangle_t$$

$$+ a_{i+1}(f_{i-1}-f_i)\mathcal{W}_{i-1,\,i}\langle \eta_{i-1}\eta_i \eta_{i+1}\rangle_t \; . \tag{2.35}$$

By using Eq. (2.30) and by neglecting all correlators except $\langle \eta_i \eta_{i+1}\rangle$, in the stationary state, we get

$$C(f_{i+1}-f_i) = b_i \langle \eta_i \eta_{i+1}\rangle \; , \tag{2.36}$$

with

$$b_i = a_i \mathcal{W}_{i+1,\,i+2} + a_{i+1}\mathcal{W}_{i-1,\,i} \; , \tag{2.37}$$

and finally we obtain

$$\lambda_i = C\frac{(f_{i+1}-f_i)^2}{b_i} \; , \tag{2.38}$$

$$\langle\langle \lambda_i \rangle\rangle = C\left[\frac{1}{N}\sum_{i=1}^{N}\frac{(f_{i+1}-f_i)^2}{b_i}\right] \equiv Cd \; , \tag{2.39}$$

where d is another obvious shorthand notation. By simple algebraic manipulation we get

$$f = (1 + d\langle\langle \mathcal{W}_{i,\,i+1}^{-1}\rangle\rangle^{-1})^{-1} \; , \tag{2.40}$$

which holds for any periodic model, i.e., any value of N, and also for the disordered system, as was discussed at the end of Sec. II B.

III. APPLICATION TO A SITE-DISORDERED MODEL

We illustrate the general result, Eq. (2.40), with a chain with two types of sites, A and B, having different potential energies ε_A and ε_B. The simplest ordered case is that of the $ABAB$ chain, where $N=2$. This is the only known model for which the effect of correlations was exactly accounted for.[5] We shall name it the Richards model. We shall also consider some other ordered models and the random one.

Let z denote the fugacity,

$$z = \exp(\beta\mu) \; , \tag{3.1}$$

and let

$$E_{A,B} = \exp(\beta\varepsilon_{A,B}) \; . \tag{3.2}$$

The Fermi functions are given by

$$f_{A,B} = \frac{z}{z+E_{A,B}} \; . \tag{3.3}$$

If N_A and N_B are the number of A and B sites per elementary cell,

$$N_A + N_B = N \; , \tag{3.4}$$

then the concentrations of A and B sites are

$$p_{A,B} = \frac{N_{A,B}}{N} \tag{3.5}$$

and the concentration of particles is given by

$$c = p_A f_A + p_B f_B \; . \tag{3.6}$$

Equation (3.6) is solved to obtain the fugacity in terms of concentration:

$$z = (1-c)^{-1}\{cE_2 - E_1$$
$$+ [(cE_2 - E_1)^2 + c(1-c)E_A E_B]^{1/2}\} \; , \tag{3.7}$$

where

$$E_1 = \tfrac{1}{2}(p_A E_A + p_B E_B) \; , \tag{3.8}$$

$$E_2 = \tfrac{1}{2}(E_A + E_B) \; . \tag{3.9}$$

The transition rates must obey the detailed-balance condition, but are otherwise arbitrary. We make the following customary choice:

$$W_{i,j} = W \exp\left[\frac{\varepsilon_j - \varepsilon_i}{2kT}\right] \; . \tag{3.10}$$

Thus, we have

$$\mathcal{W}_{AA} = Wf_A(1-f_A) = Wa_A \; , \tag{3.11}$$

$$\mathcal{W}_{BB} = Wa_B \; , \tag{3.12}$$

$$\mathcal{W}_{AB} = W_{AB}f_A(1-f_B) = (\mathcal{W}_{AA}\mathcal{W}_{BB})^{1/2} \; . \tag{3.13}$$

In the case of the Richards model, where the only correlators that have a nonzero contribution to the conductivity are the NN ones,[5] Eq. (2.40), which is generally an approximate formula, gives the exact result

$$f_R = \left[1 + \frac{(f_A - f_B)^2}{a_A + a_B}\right]^{-1} \; . \tag{3.14}$$

Let us calculate $\langle\langle \mathcal{W}_{i,\,i+1}^{-1}\rangle\rangle^{-1}$ and d for the random model. If by p_{AA} we denote the probability of finding an AA cluster in the chain, and we make similar notations for the probabilities of other clusters, we have

$$p_{AA} = p_A^2, \quad p_{BB} = p_B^2, \quad p_{AB} = p_{BA} = p_A p_B \; . \tag{3.15}$$

The same factorization holds for greater clusters, such as

$$p_{AAAA} = p_A^4 \; , \tag{3.16}$$

and other similar relations. By Eq. (3.15), we get

$$\langle\langle \mathcal{W}_{i,\,i+1}^{-1}\rangle\rangle_{\text{random}}^{-1} = \left[\frac{p_A^2}{\mathcal{W}_{AA}} + \frac{p_B^2}{\mathcal{W}_{BB}} + \frac{2p_A p_B}{\mathcal{W}_{AB}}\right]^{-1} \; , \tag{3.17}$$

and by Eq. (3.16), we get

$$d_{\mathrm{random}} = 2(f_A - f_B)^2 p_A p_B \left[\frac{p_A^2}{b_{ABAA}} + \frac{p_B^2}{b_{BABB}} + \frac{p_A p_B}{b_{ABAB}} + \frac{p_A p_B}{b_{AABB}} \right] , \tag{3.18}$$

where we have used the notation of Eq. (2.37) with special indices for clusters of four sites:

$$b_{ABAA} = a_B \mathcal{W}_{AA} + a_A \mathcal{W}_{AB}, \quad b_{ABAB} = (a_A + a_B) \mathcal{W}_{AB} , \tag{3.19}$$

$$b_{BABB} = a_A \mathcal{W}_{BB} + a_B \mathcal{W}_{AB}, \quad b_{AABB} = a_A \mathcal{W}_{BB} + a_B \mathcal{W}_{AA} .$$

For the sake of simplicity, we will take $p_A = p_B = 0.5$ from now on.

We also consider a simple periodic model, with $N = 4$, namely, the one having $AABB$ as the elementary cell. For this case, we get the same probabilities of two-site clusters as in Eq. (3.15), and thus the same MF result. The correlation factors of the three models considered up to now are given in Fig. 3, as functions of concentration. For this particular illustration, the energies were chosen so that $E_B = 10E_A$. One would be tempted to draw the conclusion that disorder softens the effect of correlations. This would be a hasty and incorrect statement. First of all, Eq. (2.40) is only an approximate formula, and neither the result for the random chain, nor the $AABB$ result is exact, although we believe that they are reasonably close to the true values (the argument being the success of the first nontrivial approximation in more complicated hopping systems[8,10,13]). Second, but more important, we have easily found some ordered models with a higher value of the correlation factor than the random one, an aspect that will be discussed below.

Let us take the $AABB$ model and "scale" it thus: $AAABBB$ ($N=6$), $AAAABBBB$($N=8$), and so on. For $N = 2n$, we get

$$\langle\!\langle \mathcal{W}_{i,i+1}^{-1} \rangle\!\rangle^{-1} = 2n \left[\frac{n-1}{\mathcal{W}_{AA}} + \frac{n-1}{\mathcal{W}_{BB}} + \frac{2}{\mathcal{W}_{AB}} \right]^{-1} , \tag{3.20}$$

$$d = \frac{(f_A - f_B)^2}{n b_{AABB}} . \tag{3.21}$$

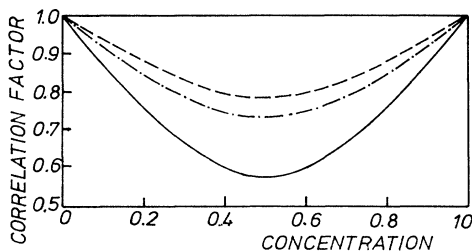For increasing values of n, d becomes vanishingly

FIG. 3. The correlation factor of the conductivity vs concentration for three-dimensional models with two types of sites: the random chain ($- - -$), the $AABB$ chain ($-\cdot-\cdot-\cdot$), and the Richards model ($\longrightarrow$). The energies were chosen so that $\exp[\beta(\varepsilon_B - \varepsilon_A)] = 10$.

small, and so the correlation factor can grow arbitrarily high towards the limiting value 1, and the system becomes uncorrelated for $n \to \infty$. This is not surprising, since it is the AB bonds that are important for the correlations to be effective.

Let us then examine one particular class of periodic systems, namely, those with a fixed value of the concentration of AB bonds. We take

$$p_{AB} = p_{BA} = 0.25 \tag{3.22}$$

as for the random chain, Eq. (3.15). This restriction leads to a more proper comparison between order and disorder. It is interesting to note that from Eq. (3.22) it necessarily follows that

$$p_{AA} = p_{BB} = 0.25 \tag{3.23}$$

and therefore all these systems have the same $\langle\!\langle \mathcal{W}_{i,i+1}^{-1} \rangle\!\rangle^{-1}$ as the random one. The correlation factor is determined by the distribution of four-site clusters, i.e., by the values of b_i, Eq. (3.19). For $c < 0.5$ and $\varepsilon_A < \varepsilon_B$, we have

$$f_A > f_B , \tag{3.24a}$$

$$a_A > a_B . \tag{3.24b}$$

For $c > 0.5$ the inequality (3.24b) inverts, but the following discussion holds by analogy, and so we shall consider Eqs. (3.24) to hold true. Then, for Eqs. (3.19), which are immediately written as

$$b_{ABAA} = \sqrt{a_A a_B}(a_A + \sqrt{a_A a_B})W ,$$
$$b_{BABB} = \sqrt{a_A a_B}(a_B + \sqrt{a_A a_B})W ,$$
$$b_{ABAB} = \sqrt{a_A a_B}(a_A + a_B)W , \tag{3.25}$$
$$b_{AABB} = 2a_A a_B W ,$$

the following inequalities are evident:

$$b_{ABAA} > b_{ABAB} > b_{AABB} > b_{BABB} . \tag{3.26}$$

Another relation which is important for the following considerations is readily shown:

$$\frac{1}{b_{ABAA}} + \frac{1}{b_{AABB}} = \frac{2}{b_{AABB}} . \tag{3.27}$$

The ordered systems which have equal concentrations of AA, BB, and AB clusters, have $N = 4n$. For $n = 1$, the only model is the $AABB$ one, which, by Eqs. (3.26) and (3.27), is seen to have a higher value of d and consequently a lower f than the disordered chain. For $n = 2$, there are three such systems: $AAABABBB$, $AAABBABB$, and $BBBAABAA$. For the first one, we obtain the same value of d as in the random case, and thus an equal f (and an equal σ); for the other two, we get, by Eq. (3.26),

$$d_{AAABBABB} = \frac{(f_A - f_B)^2}{4} \left[\frac{1}{b_{BABB}} + \frac{1}{b_{AABB}} \right] > d_{\text{random}} ,$$

(3.28)

$$d_{BBBAABAA} = \frac{(f_A - f_B)^2}{4} \left[\frac{1}{b_{ABAA}} + \frac{1}{b_{AABB}} \right] < d_{\text{random}} .$$

(3.29)

In the frame of the present approximation, the correlation factor depends essentially on the relative concentrations of four-site clusters. While in the random chain these clusters appear in equal proportions, it is clear that one can devise ordered systems in which clusters with smaller or greater b's are dominant and so obtain smaller or larger correlation factors, respectively. Thus, one can say that disordered chains do not occupy privileged positions among one-dimensional correlated hopping systems.

Let us note that all the cases analyzed indicate that the exactly soluble Richards model does occupy such a special position. Due to the fact that this model has only AB bonds, all $(f_{i+1} - f_i)^2$ factors in Eq. (2.39) have a nonvanishing value—in fact, the *same* value—and the d factor in Eq. (2.40) seems to be maximal, which leads to a minimal value of f.

IV. SUMMARY AND CONCLUSIONS

We calculated the hopping conductivity of a one-dimensional lattice gas that has no other interactions except for the hard-core repulsion.

By considering stationary flow on a periodic chain, in the presence of a uniform electric field, the MF conductivity as well as the first correction due to dynamic correlations were obtained. The results were easily extended to nonperiodic chains.

While the MF conductivity of a one-dimensional disordered system has been known for quite a long time,[2] the present paper presents an attempt to estimate the influence of correlations for such systems. Calculations were made by neglecting all η correlation functions except the NN ones: $\langle \eta_i \eta_{i+1} \rangle$, $i = 1, 2, \ldots, N$, η_i being the deviation of the occupation number n_i from its equilibrium value.

The general formula that was obtained for the correlation factor f, Eq. (2.40), was discussed for the particular case of a chain with two site energies. Several periodic models as well as the random one were considered. We found periodic systems with both stronger and weaker correlation effects than the completely random chain. Therefore it is clear that the latter occupies no special position as far as the correlations are concerned. On the other hand, numerical evidence suggests that in the Richards model their effect is maximal.

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[12]This stems from the definition of v as the center of mass velocity:

$$\mathbf{v} = \frac{d}{dt} \left[\sum_i \langle n_i \rangle_t \mathbf{x}_i \Big/ \sum_i \langle n_i \rangle_t \right] ,$$

where $\mathbf{x}_i$ is the position of site i (in our one-dimensional case $x_i = ia$) and $\sum_i \langle n_i \rangle_t = N_p$. The time derivative of $\langle n_i \rangle_t$ is given in Refs. 5 and 11, and, using our notations, takes the form of Eq. (2.10).

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