

Hopping conductivity of the interacting honeycomb lattice gas

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The hopping conductivity of the honeycomb lattice gas with nearest-neighbor repulsion is calculated by a stationary-flow formalism. The necessary static correlation functions are evaluated in the Bethe-Peierls approximation. The dynamic correlations are considered in the first nontrivial approximation. The correlation function is obtained for several temperatures.

I. INTRODUCTION

The lattice gas has been intensively used as a model for charge and mass transport in condensed matter. The past two decades have witnessed a growing interest in highly defective solids such as superionic conductors and metal hydrides (see Refs. 1 and 2, and references therein). The modeling of these materials must take into account interactions between the diffusing particles which are available in high concentrations. Transport in several types of interacting lattice gases has been studied through various approaches, such as the path-probability method,^{3,4} the rate equation formalism⁵⁻¹¹ and Monte Carlo simulations¹²⁻¹⁵ (see also Refs. 16 and 17, and references therein). Some exact results were obtained only for one-dimensional systems.⁵⁻⁷ The theoretical investigation of two- and three-dimensional lattices involves approximations, as in the case of equilibrium properties.

In a previous work¹⁸ we studied the infinite nearest-neighbor repulsion in the square lattice gas. One would like to weaken the strength of the interaction but this would lead to tedious calculations in the case of the square lattice, which involved long enough formulas even for the somewhat simple case of the extended-hard-core repulsion.

We found that the formulas are no longer too complex in the case of the honeycomb lattice, which has the obvious advantage of having the smallest coordination number of all high-dimensional lattices, namely $Z_c = 3$. In the present paper we calculate the hopping conductivity on the honeycomb lattice, for particles that interact only at nearest-neighbor distance. Instead of varying the strength of the interaction we shall let the temperature take several values. The case of the extended-hard-core is obtained at zero temperature, while the noninteracting gas is found for $T \rightarrow \infty$.

The honeycomb lattice gas with nearest-neighbor repulsion has already been studied in connection with β and β'' aluminas, in a series of papers which started with the work of Sato and Kikuchi.³ Their model and the path-probability method have since been improved. The most recent work on the subject is that of Collin and co-workers^{19,20} where an extensive discussion is made, taking into account three-dimensional effects.

The thermal equilibrium properties of our model are determined by the same Hamiltonian as the one used by Sato and Kikuchi and others. Concerning the transport properties, it is known that the jump rates must satisfy detailed balance in order to ensure evolution towards equilibrium, but they are not uniquely specified by this condition. Thus, for a given system with a given Hamiltonian, they remain somewhat arbitrary (see extensive discussion in Refs. 7 and 17). We have favored the type of rates chosen by Kehr, Binder, and co-workers,¹⁷ because, unlike those used by Sato and Kikuchi, these include the extended-hard-core interaction as a limit case.

In Sec. II the Bethe-Peierls approximation (BPA) is used to study the static correlation functions of the model. The vacancy availability factor is calculated and compared with the Monte Carlo results of Murch and Thorn.¹² A phase diagram in the concentration-temperature plane is also derived within the BPA and compared to previous results.

The conductivity and its correlation factor are calculated in Sec. III with a steady-state approach from Richards.²¹ The results are summarized and discussed in Sec. IV.

II. STATIC CORRELATIONS

We consider a system of N_p identical particles on a honeycomb lattice with N equivalent sites. There is a nearest-neighbor (NN) repulsion between particles. The system is described by the set of occupation numbers $\{n_i\}_i$, n_i taking the value 0 or 1 if the site i is empty or occupied, respectively. The Hamiltonian of the problem is given by

$$\mathcal{H}(\{n_i\}_i) = \epsilon \sum_{i=1}^N n_i + \frac{1}{2} \mathcal{J} \sum_{i,j=1}^N n_i n_j \quad (2.1)$$

where ϵ is the energy of one site, $\mathcal{J} > 0$ is the interaction energy and the second sum is restricted to the NN sites.

At equilibrium, with no external fields, translational invariance holds and the mean value of n_i in the grand-canonical ensemble is equal to the concentration of particles:

$$\langle n_i \rangle_0 = \frac{1}{Z} \text{Tr}(n_i e^{-\beta(\mathcal{H} - \mu N)}) = c = \frac{N_p}{N}, \quad (2.2)$$

where the subscript 0 indicates an equilibrium average and

$$Z = \text{Tr}(e^{-\beta(\mathcal{H}-\mu N)}) \\ = \sum_{\{n_i\}} \exp \left[-\beta \left[\sum_i (\varepsilon - \mu) n_i - \frac{1}{2} \mathcal{J} \sum_{ij} n_i n_j \right] \right] \quad (2.3)$$

is the grand-canonical partition function.

In order to evaluate the static correlation functions, we shall use the Bethe-Peierls approximation (BPA), which seems to be the best tool for this purpose (counting out computer simulations), as was discussed by Froböse and Jäckle¹⁵ for the extended-hard-core square lattice gas.

In the BPA the lattice is replaced by a small cluster of adjoining sites. We consider that in Fig. 1. The central site has the "bulk" chemical potential μ , while the other sites have chemical potentials of *a priori* different values μ_1, μ_2, μ_3 in order to account for the influence of the lattice sites outside the cluster. The respective fugacities are

$$z = \exp[-\beta(\varepsilon - \mu)] , \\ z_i = \exp[-\beta(\varepsilon - \mu_i)] , \quad i = 1, 2, 3 . \quad (2.4)$$

Considering c as a parameter the z 's are determined by Eq. (2.2):

$$c = \langle n_0 \rangle_0 = \langle n_1 \rangle_0 = \langle n_5 \rangle_0 = \langle n_{10} \rangle_0 . \quad (2.5)$$

Taking the fugacity rather than the chemical potential as an independent variable, the temperature appears only in conjunction with the repulsion strength, \mathcal{J} . Therefore we introduce the reduced temperature by

$$T^* = (\beta \mathcal{J})^{-1} . \quad (2.6)$$

Making the following notations:

$$E = \exp \left[-\frac{1}{T^*} \right] , \quad (2.7)$$

$$Z_0 = (z_2 + 1)^2 + z_3(z_2 E + 1)^2 , \quad (2.8)$$

$$Z_1 = (z_2 E + 1)[(z_2 + 1) + z_3(z_2 E^2 + 1)] ,$$

$$Z_2 = (z_2 E + 1)^2 + z_3(z_2 E^2 + 1)^2 ,$$

the grand-canonical partition function of the cluster is

$$Z_{cl} = (z + 1)Z_0^3 + 3z_1(zE + 1)Z_0Z_1^2 \\ + 3z_1^2(zE^2 + 1)Z_1^2Z_2 + z_1^3(zE^3 + 1)Z_2^3 . \quad (2.9)$$

Equations (2.5) become

$$c = z \frac{\partial \ln Z_{cl}}{\partial z} , \\ c = \frac{z_1}{3} \frac{\partial \ln Z_{cl}}{\partial z_1} , \\ c = \frac{z_2}{6} \frac{\partial \ln Z_{cl}}{\partial z_2} , \\ c = \frac{z_3}{3} \frac{\partial \ln Z_{cl}}{\partial z_3} . \quad (2.10)$$

Equations (2.10) are solved numerically for different values of $E \in [0, 1]$. For $E = 0$ the trivial case of infinite temperature or, equivalently, the noninteracting lattice gas is found, Eqs. (2.10) becoming exactly soluble. For $E = 1$ we get the case of zero temperature or the extended-hard-core interaction. The values $T^* = 0.3$, $T^* = 0.5$, $T^* = 1.0$ are also considered. The results for the fugacity z are presented in Fig. 2.

We are in the position to compute any correlator which involves sites situated not farther apart than those in our BPA cluster. For illustration, we give in Fig. 3 the values obtained for the vacancy availability factor, defined as the probability of finding a given empty site near a given occupied one:

$$V = \frac{\langle n_0(1 - n_1) \rangle_0}{c} = 1 - \frac{\langle n_0 n_1 \rangle_0}{c} . \quad (2.11)$$

The results for V are in good agreement with the Monte Carlo values obtained by Murch and Thorn¹² (the deviation from computer experiments being less than 1% for all concentrations and temperatures considered), which shows the reliability of the BPA.

The accuracy of the BPA can also be judged by examining the results on the separation line between the disordered and the ordered phases of the system. At low temperatures and concentrations around 0.5, the system is found in an ordered state in which one of the two sublattices made up of next-nearest-neighbour sites is preferentially occupied.^{3,12} For $c = 0.5$ the transition temperature is exactly known, $T^* = 0.380$.²² A phase diagram obtained within the cluster variation approximation (CVA) was given by Sato and Kikuchi.³

The onset of order, as well as static properties of the ordered state may be derived by a modified BPA in which the number of equations is roughly twice that of the disordered case.¹⁵ We have calculated the critical concentrations for several temperatures as follows. A cluster in which the two sublattices are symmetrically represented was chosen as in Fig. 4. Excepting the two central sites that have identical fugacity z , peripheral sites have different fugacities $z_{iA} \neq z_{iB}$, $i = 1, 4$, if they belong to sublattice A or B , respectively. The grand-canonical parti-

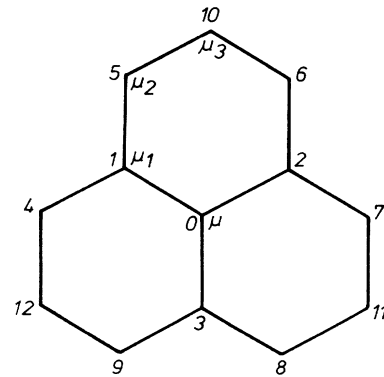


FIG. 1. The cluster representing the lattice in the Bethe-Peierls approximation. The values of the chemical potential are indicated.

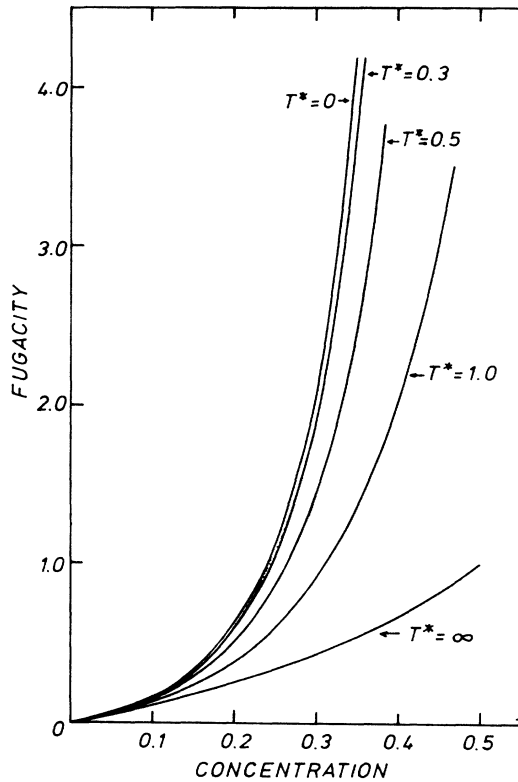


FIG. 2. Fugacity vs concentration for several values of the reduced temperature, in the Bethe-Peierls approximation.

tion function of the cluster was calculated and a system of ten coupled equations similar to Eqs. (2.9) was written, with different values of the concentration on the two sublattices:

$$\begin{aligned} c_A &= \langle n_A \rangle = \langle n_{iA} \rangle, \\ c_B &= \langle n_B \rangle = \langle n_{iB} \rangle, \quad i = 1, 2, 3, 4. \end{aligned} \tag{2.12}$$

The mean concentration

$$c = \frac{c_A + c_B}{2} \tag{2.13}$$

being given, the unknown parameters for Eqs. (2.12) are the nine fugacities and the difference between the concentrations:

$$\eta = c_A - c_B. \tag{2.14}$$

Rather than write Eqs. (2.12) in detail and solve them numerically, we used an equivalent approach. Consider the function

$$\begin{aligned} F &= \frac{1}{Z_{cl}^{A,B}} (z_A z_{1A}^2 z_{2A}^2 z_{3A} z_{4A}^2)^{c+\eta/2} \\ &\quad \times (z_B z_{1B}^2 z_{2B}^2 z_{3B} z_{4B}^2)^{c-\eta/2}. \end{aligned} \tag{2.15}$$

It is easily seen that Eqs. (2.12) are equivalent to obtaining that value of η for which, at a given c , the maximum of F is obtained when $z_A = z_B$. By using a maximization subroutine, we have plotted $z_A - z_B$ versus η for different concentrations at given temperature, looking for a zero. The critical concentration was determined as the lowest value at which the two symmetrical solutions $\eta_1 = -\eta_2 \neq 0$ appear beside the permanent $\eta = 0$ solution. The results are given in Fig. 5, in comparison with the CVA phase diagram. It is seen that although still far from the true separation line (out of which one point is known exactly) our curve is closer to it than the CVA one. At $c = 0.5$, our $T_{BPA}^* = 0.4212$ lies between the exact $T^* = 0.380$ and that of Ref. 3, $T_{CVA}^* = 0.45512$.

It is known that in the ordered phase the mobility of particles becomes very low. Since the main purpose of this paper is the calculation of conductivity, we shall restrict all further considerations to the disordered state.

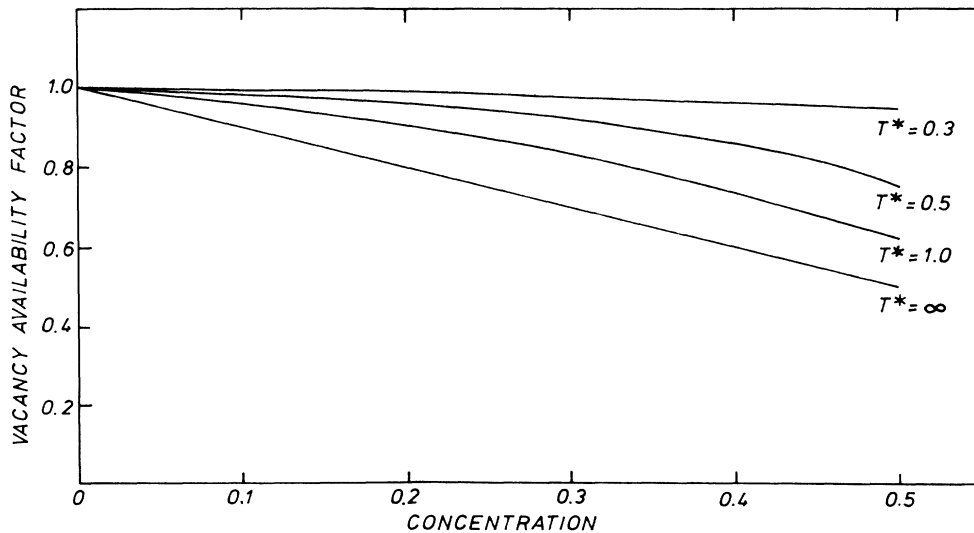


FIG. 3. Vacancy availability factor vs concentration for several values of the reduced temperature, in the Bethe-Peierls approximation.

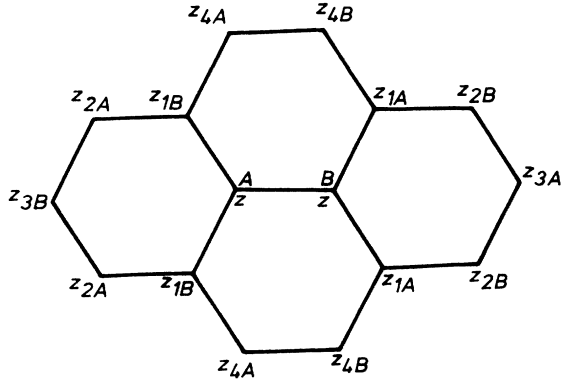


FIG. 4. The cluster used for deriving the phase diagram in the Bethe-Peierls approximation. The different values of the fugacities corresponding to the two sublattices A and B are indicated.

III. STATIONARY FLOW

We now make use of a steady-state approach developed by Richards²¹ to evaluate the conductivity of our model. The lattice of N sites is periodically repeated to cover the whole plane so that a stationary flow is possible without sources of particles. The sites are labeled (i, j) with i and j corresponding to the x and y axis, respectively (see Fig. 6). The particles, having the electrical charge e , can jump to a NN vacant site with a jump rate that depends (symmetrically) on the occupancy of the NN's of both the initial and the final site. Thus, the jump rate from site (i, j) to site $(i + 1, j)$ will be:

$$W_{(i,j),(i+1,j)} = W n_{(i,j)} (1 - n_{(i+1,j)}) \times \left[1 + \tanh \frac{\beta \delta H_{(i,j)(i+1,j)}}{2} \right], \quad (3.1)$$

$$W_{10} = W n_1 (1 - n_0) \left[1 + \tanh \frac{\beta \delta}{2} (n_4 + n_5 - n_2 - n_3) + \left[\tanh \beta \delta - 2 \tanh \frac{\beta \delta}{2} \right] [n_4 n_5 (1 - n_2 - n_3) - n_2 n_3 (1 - n_4 - n_5)] \right]. \quad (3.2)$$

The infinite interaction limit gives

$$W_{10} \xrightarrow{T^* \rightarrow 0} W n_1 (1 - n_0) (1 - n_2) (1 - n_3) (1 - n_4) (1 - n_5). \quad (3.3)$$

In Eq. (3.3) the factors $(1 - n_0)(1 - n_4)(1 - n_5)$ are superfluous because $n_1 = 1$ leads to $n_0 = n_4 = n_5 = 0$, so that we have

$$W_{10}|_{T^*=0} = W n_1 (1 - n_2) (1 - n_3). \quad (3.4)$$

In the presence of an electric field $\mathcal{E} = \mathcal{E} \mathbf{e}_x$, the difference in energy between two NN sites in the $(1, \pm \frac{1}{2})$

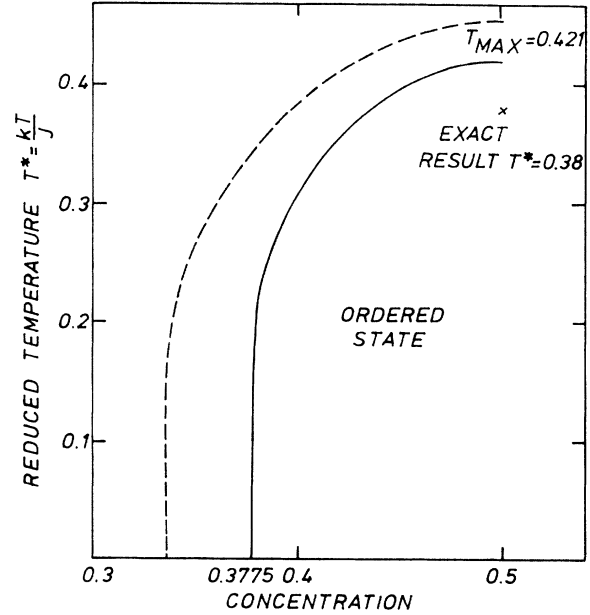


FIG. 5. The separation line between order and disorder in the concentration-temperature plane, derived within the Bethe-Peierls approximation (solid line). The exact critical temperature $T^* = 0.38$ for $c = 0.5$ is indicated. The dashed curve represents the same line obtained in Ref. 3 by the cluster variation approximation.

where δH is the difference in energy between the configurations before and after the jump and W is the jump rate when the interaction is zero.

This choice, which is that made by Kehr, Binder, and their group¹⁷ coincides for $E = 1$ with the one that is naturally made in the case of the extended-hard-core model.^{15,18}

The explicit dependence of the jump rate on the occupation numbers, with the notations in Fig. 1, is given by

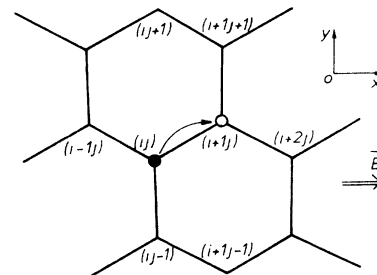


FIG. 6. The jump of a particle from site (ij) to site $(i + 1j)$. The axes and the direction of the field are indicated.

directions is $e\mathcal{E}l$ where

$$l = \frac{a\sqrt{3}}{2}, \quad (3.5)$$

a being the NN distance. In order to satisfy detailed balance, the rates for jumps in the above-mentioned directions are modified symmetrically as follows:

$$W_{(i,j),(i\pm 1,j)}^{\mathcal{E}} = W_{(i,j),(i\pm 1,j)}(1\pm\Delta) \quad (3.6)$$

with

$$\Delta = \frac{e\mathcal{E}l}{2kT}. \quad (3.7)$$

Equation (3.6) is written only up to first order in \mathcal{E} which is sufficient for the calculation of conductivity. In the following, we will systematically discard higher-order terms.

The charge current density is given by

$$j = \frac{N_p}{N\Omega} ev = \frac{cev}{\Omega}, \quad (3.8)$$

where $\Omega = 3\sqrt{3}a^2/4$ is the area per site and v is the mean

$$v_{\text{corr}} = -lWN \left[\tanh\frac{\beta\mathcal{J}}{2} \langle \langle n_1 n_3 \rangle \rangle - \tanh\beta\mathcal{J} \langle \langle n_0 n_1 n_3 \rangle \rangle - 2 \left[\tanh\beta\mathcal{J} - 2\tanh\frac{\beta\mathcal{J}}{2} \right] \left[\langle \langle n_0 n_2 n_3 n_4 \rangle \rangle + \langle \langle n_1 n_2 n_3 n_4 \rangle \rangle + 2 \langle \langle n_0 n_1 n_2 n_4 n_5 \rangle \rangle \right] \right]. \quad (3.14)$$

The equilibrium average appears in Eq. (3.13) due to the Δ prefactor.

In Eq. (3.14) we have introduced the notation $\langle \langle f(n) \rangle \rangle$ for a new type of steady-state correlator, namely the difference between $\langle f(n) \rangle$ and its reflection towards the y axis. These symmetrized correlators will be simply called “dynamic.” We illustrate them with the first one in the right-hand side of Eq. (3.14), which plays an important role in this paper. It is denoted by ζ and it is given by

$$\zeta \equiv \langle \langle n_1 n_3 \rangle \rangle \equiv \langle n_1 n_3 \rangle - \langle n_2 n_3 \rangle. \quad (3.15)$$

From the obvious relation

$$\langle n_1 n_3 \rangle = \langle n_1 n_3 \rangle_0 + \mathcal{O}(\Delta) \quad (3.16)$$

it follows that $\zeta = \mathcal{O}(\Delta)$.

A trivial approximation for the conductivity is obtained by neglecting all dynamic correlators, i.e.,

$$v \simeq v_{\infty}. \quad (3.17)$$

This leads to the infinite-frequency conductivity:

$$\sigma_{\infty} = \frac{j_{\infty}}{\mathcal{E}} = \frac{cev_{\infty}}{\Omega} \frac{el}{2kT\Delta} = \frac{N_p e^2 l^2}{\Omega kT} \langle W_{10} \rangle_0. \quad (3.18)$$

The dynamic correlators that make the dc conductivity σ lower than σ_{∞} are all included in v_{corr} , Eq. (3.14). We shall evaluate v_{corr} in the first nontrivial approximation, following the same recipe as in Ref. 18.

velocity of the particle in the field direction in the steady state. The velocity is given by¹⁸

$$v = l \sum_{i,j} (\langle W_{(i,j),(i+1,j)}^{\mathcal{E}} \rangle - \langle W_{(i,j),(i-1,j)}^{\mathcal{E}} \rangle). \quad (3.9)$$

Equation (3.9) involves stationary-flow correlation functions which have two useful symmetry properties: they are invariant under translation and under reflection towards the field direction. For illustration, we have

$$\langle n_0 n_1 \rangle = \langle n_0 n_2 \rangle = \langle n_1 n_4 \rangle. \quad (3.10)$$

This simplifies Eq. (3.9) as follows:

$$v = lN (\langle W_{10}^{\mathcal{E}} \rangle - \langle W_{01}^{\mathcal{E}} \rangle) \quad (3.11)$$

or, explicitly,

$$v = v_{\infty} + v_{\text{corr}}, \quad (3.12)$$

where

$$v_{\infty} = 2\Delta lN \langle W_{10} \rangle_0 \quad (3.13)$$

and

The higher-order correlators may be expressed in terms of lower-order ones. This is most easily done at $T^* = 0$. If δ_i denotes the deviation of n_i from its equilibrium mean value c , a correlator of, say, four particles, can be written as

$$\langle \langle n_a n_b n_c n_d \rangle \rangle = c^2 \sum_{i,j} \langle \langle n_i n_j \rangle \rangle + c \sum_{i,j,k} \langle \langle \delta_i \delta_j \delta_k \rangle \rangle + \langle \langle \delta_a \delta_b \delta_c \delta_d \rangle \rangle, \quad (3.19)$$

where we have omitted the vanishing $\langle \langle \delta_i \rangle \rangle$, and the obvious relation

$$\langle \langle n_i n_j \rangle \rangle = \langle \langle \delta_i \delta_j \rangle \rangle \quad (3.20)$$

was used. In the first approximation, only one dynamical correlator of δ 's is retained, namely ζ which is of order two in δ :

$$\zeta = \langle \langle n_1 n_3 \rangle \rangle = \langle \langle \delta_1 \delta_3 \rangle \rangle. \quad (3.21)$$

All other products of δ 's will be neglected, so that higher-order correlators of n 's will be expressed in terms of ζ by Eq. (3.19).

While the expansion in powers of fluctuations Eq. (3.19) leads to good results in the case of the extended-hard-core¹⁸ it is not suitable for finite repulsion, a fact which is easily seen in the following example. Let us apply Eq. (3.19) to $\langle \langle n_0 n_1 n_3 \rangle \rangle$:

$$\begin{aligned} \langle \langle n_0 n_1 n_3 \rangle \rangle &= c(\langle \langle n_0 n_1 \rangle \rangle + \langle \langle n_0 n_3 \rangle \rangle + \langle \langle n_1 n_3 \rangle \rangle) \\ &\quad + \langle \langle \delta_0 \delta_1 \delta_3 \rangle \rangle \\ &= c \langle \langle n_1 n_3 \rangle \rangle, \end{aligned} \quad (3.22)$$

where $\langle \langle n_0 n_1 \rangle \rangle$ and $\langle \langle n_0 n_3 \rangle \rangle$ are zero by symmetry and $\langle \langle \delta_0 \delta_1 \delta_3 \rangle \rangle$ is neglected, as mentioned before. Equation (3.22) is incorrect because $\langle \langle n_1 n_3 \rangle \rangle$, which contains no NN sites, has a finite value in the limit $T^* \rightarrow 0$ while $\langle \langle n_0 n_1 n_3 \rangle \rangle$ should vanish. In the general case, the formula for the decomposition of a higher-order correlator which involves NN sites must be modified to include the interaction explicitly, so that all terms of the expansion vanish for infinite repulsion. Therefore the coefficient of a lower-order correlator with no NN sites must be zero at $T^* = 0$. A possible modification, which in fact will be adopted here, is to include an E factor whenever a NN bond is broken by decoupling. For illustration, we have

$$\langle \langle n_0 n_1 n_3 \rangle \rangle \simeq cE^2 \langle \langle n_1 n_3 \rangle \rangle. \quad (3.23)$$

Apart from fulfilling the above-mentioned conditions, this handling of nonequilibrium correlators is supported by some equilibrium-state arguments. First, a factor E associated with the bond to be broken is present in all terms of the formula that gives the higher-order correlation function, while it is no longer present in the formula for the lower-order one. Also, the approximation works well in the case of the one-dimensional lattice for which exact static results are available. In addition, the numerical results obtained by BPA are also a good test for this type of approximation.

By expressing all higher-order correlators in terms of ζ as in Eq. (3.23), we get the approximate formula

$$v_{\text{corr}} = -lWNQ\zeta, \quad (3.24)$$

where

$$\begin{aligned} Q &= \tanh \frac{\beta\mathcal{J}}{2} - cE^2 \tanh \beta\mathcal{J} \\ &\quad + 2E^2 c^2 (1 - 2E + 2E^2 c) \left[\tanh \beta\mathcal{J} - 2 \tanh \frac{\beta\mathcal{J}}{2} \right]. \end{aligned} \quad (3.25)$$

We are left with the task of evaluating ζ . For this purpose, we write down the rate equation describing the evolution of $\langle n_1 n_3 \rangle_t$. The jumps that contribute to its decrease are given in Fig. 7. The reverse jumps will increase $\langle n_1 n_3 \rangle_t$, and we get

$$\begin{aligned} \frac{d}{dt} \langle n_1 n_3 \rangle_t &= -\langle W_{30}^6 n_1 \rangle - \langle W_{38}^6 n_1 \rangle - \langle W_{39}^6 n_1 \rangle \\ &\quad - \langle W_{10}^6 n_3 \rangle - \langle W_{14}^6 n_3 \rangle - \langle W_{15}^6 n_3 \rangle + \dots, \end{aligned} \quad (3.26)$$

where the ellipsis represents terms for reverse jumps.

A similar equation is written for $\langle n_2 n_3 \rangle_t$ and the difference between the two relations is taken, in the stationary flow state when both left-hand sides vanish. The

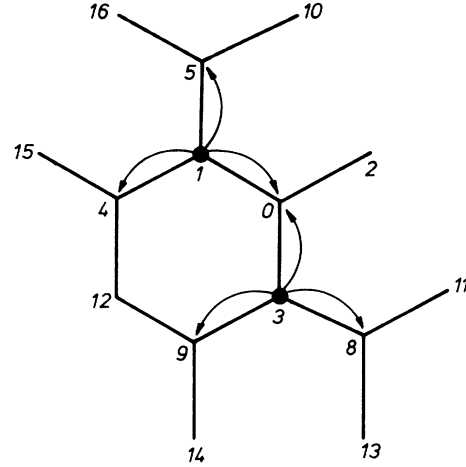


FIG. 7. Jumps contributing to the decrease of $\langle n_1 n_3 \rangle_t$.

equation obtained is too long to be given here. We shall only describe the calculations that are straightforward and similar to the treatment of the formula for v , Eq. (3.11). The terms with a Δ factor are evaluated in the equilibrium ensemble within the BPA and the dynamic correlators are again expressed in terms of ζ . We get a self-consistent equation for ζ , which leads to

$$\zeta = \frac{2\Delta\zeta_0}{6 - 2 \tanh(\beta\mathcal{J}/2) + A - B}, \quad (3.27)$$

where ζ_0 is a long sum of equilibrium correlators up to the fifth order and

$$A = c(7E^2 + 5E - 5 - 12E^3 + 6E^2 c) \tanh \frac{\beta\mathcal{J}}{2}, \quad (3.28)$$

$$\begin{aligned} B &= c[E^2 + c(3E^3 + E^2 - 2) - c^2(6E^4 + E^3 - 9E^2 - 5E) \\ &\quad - c^3(8E^5 + 10E^4)] \left[\tanh \beta\mathcal{J} - 2 \tanh \frac{\beta\mathcal{J}}{2} \right]. \end{aligned}$$

The conductivity correlation factor is given by

$$f = \frac{\sigma}{\sigma_\infty} = \frac{v}{v_\infty} = 1 + \frac{v_{\text{corr}}}{v_\infty} = 1 - \frac{Q}{\langle W_{10} \rangle_0} \frac{\zeta}{2\Delta}. \quad (3.29)$$

The results for f are shown in Fig. 8. It is seen that for low temperature f vanishes at some concentration below the critical one. Perhaps by pushing the degree of approximation further, namely by retaining more than one dynamic correlator, the value of f would be finite at the critical concentration, as the one obtained by Murch and Thorn.¹³ However, the comparison is not adequate because of the different choice of jump rates. At high temperatures the disordered phase is stable at all concentrations. Therefore, the conductivity is known to be invariant under the change of particles into vacancies, namely of c into $1 - c$. This is why only the interval $0 \leq c \leq 0.5$ was investigated.

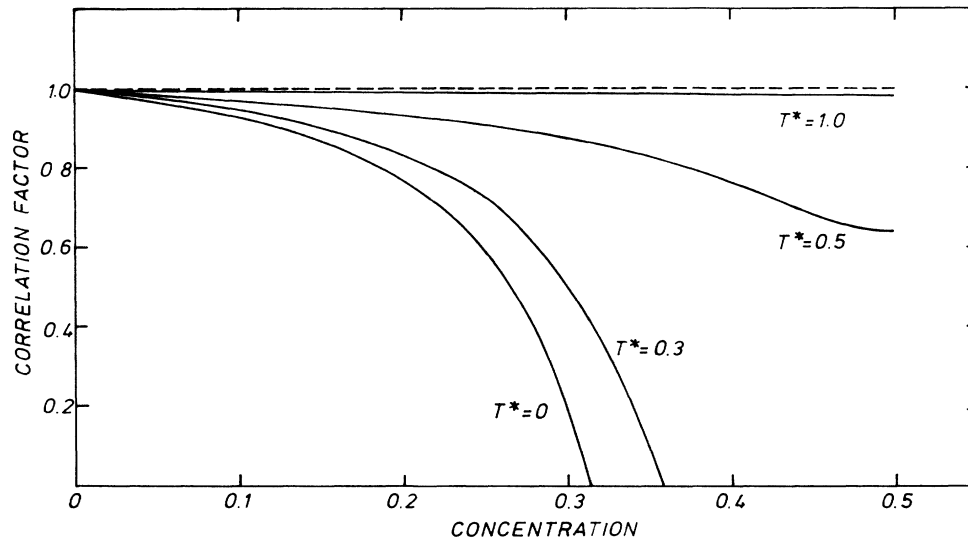


FIG. 8. The correlation factor of the conductivity vs concentration for several values of the reduced temperature.

IV. SUMMARY AND CONCLUSIONS

We have studied the honeycomb lattice gas with nearest-neighbor repulsion with the purpose of calculating the correlation factor of the conductivity, defined as the ratio between the dc and the infinite-frequency conductivities. Both static and dynamic correlation functions, i.e., averages of products of occupation numbers, were involved in the calculation.

The static properties of the model (which had previously been studied by Monte Carlo as well as theoretical approaches) were considered within the BPA. The results were compared with previous ones. The BPA is in good agreement with Monte Carlo regarding the vacancy availability factor which is of order 2 in the occupation numbers. The separation line between the disordered and the ordered phases in the concentration-temperature plane also indicated the accuracy of the BPA.

The dynamic correlators were treated in the first non-trivial approximation, in a way similar to Ref. 18. Thus, all higher-order correlation functions in the steady state were expressed in terms of the most important one,

namely ζ , Eq. (3.15). In this way, a self-consistent equation for ζ was obtained. The correlation factor of the conductivity was expressed in terms of static correlators and thus calculated numerically in the BPA. The results are different from previous computer experiments because of the different choice made for the jump rates. However, some qualitative aspects are the same. The correlation factor is a symmetric function of concentration around the value 0.5 for high temperatures when the equilibrium state is disordered at all concentrations. At low temperature it vanishes when the concentration approaches the critical values at which a phase transition to an ordered state occurs. The advantage of our jump rates is the possibility of investigating the extended-hard-core interaction, or, equivalently, the zero-temperature case as a limit of the general model.

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