

Particle kinetics on one-dimensional lattices with inequivalent sites

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A study is made of a stochastic model of particle kinetics on a one-dimensional lattice with inequivalent sites. Hard-core interactions between indistinguishable particles are incorporated by forbidding multiple occupancy of a site. An exact solution of the rate equations is obtained in the equivalent site limit. An analysis of the general case is carried out using the linearized rate equations. Approximate expressions for the conditional probabilities are derived and compared with the solutions obtained by numerical integration of the corresponding nonlinear equations. An alternative approach based on the master operator is also investigated.

I. INTRODUCTION

Although random-walk problems involving a single particle have been extensively studied in physical¹ and mathematical² contexts, comparatively little work has been done on particle kinetics in interacting systems. In this paper we report the results of a study of the rate equations associated with one of the simpler of the many-particle problems. We treat a one-dimensional stochastic model with finite concentrations of indistinguishable particles. Hard-core interactions between particles are incorporated by forbidding transitions to occupied sites.

As a generalization of the standard model, which is suggested by recent nuclear-relaxation studies,^{3,4} we divide the lattice into two interpenetrating sublattices ($ABAB\cdots$) characterized by different interlattice transition rates, W_{AB} and W_{BA} . If we define $P_i^A(t)$ [$P_i^B(t)$] to be the probability that site i which is on the A (B) sublattice is occupied at time t we can write the rate equations governing the kinetics in the form

$$\frac{dP_i^A(t)}{dt} = -W_{AB}P_i^A(t)[2 - P_i^B(t) - P_{i-1}^B(t)] + W_{BA}[1 - P_i^A(t)][P_i^B(t) + P_{i-1}^B(t)], \quad (1)$$

$$\frac{dP_i^B(t)}{dt} = -W_{BA}P_i^B(t)[2 - P_i^A(t) - P_{i+1}^A(t)] + W_{AB}[1 - P_i^B(t)][P_i^A(t) + P_{i+1}^A(t)]. \quad (2)$$

The restriction on multiple occupancy is incorporated through the factors $(2 - P_i - P_{i+1})$ and $(1 - P_i)$ in the first and second terms, respectively, on the right-hand sides of (1) and (2). Also, in obtaining solutions to (1) and (2) we make the assumption that the number of sites N is sufficiently large so that boundary effects can be neglected.

In Sec. II we analyze the general features of the model, while in Sec. III we study two limiting cases which are of particular interest. In the first

of these we take $W_{AB} = W_{BA}$ so that the sublattices are equivalent. The second case corresponds to a half-filled band, i.e., the number of particles is equal to one half the number of sites. Further aspects of our results are discussed in Sec. IV.

II. ANALYSIS

When $W_{AB} \neq W_{BA}$ the equilibrium occupation probabilities of the two sublattices, $\langle P_A \rangle$ and $\langle P_B \rangle$, will differ. We can derive a detailed balance equation relating $\langle P_A \rangle$ to $\langle P_B \rangle$ by setting the left-hand side of Eqs. (1) of (2) equal to zero. We find

$$W_{AB}\langle P_A \rangle(1 - \langle P_B \rangle) = W_{BA}\langle P_B \rangle(1 - \langle P_A \rangle). \quad (3)$$

A formal solution to Eqs. (1) and (2) can be obtained using operator techniques developed for the kinetic Ising model.^{5,6} However, as shown in the Appendix the resulting expressions for the expectation values are exceedingly complicated and defy simple evaluation and interpretation. An alternative approach, which is useful for studying the dynamics near equilibrium, is based on linearization with respect to the deviations

$$P_i^A(t) - \langle P_A \rangle \equiv U_i^A(t)$$

and

$$P_i^B(t) - \langle P_B \rangle \equiv U_i^B(t).$$

The linearized equations take the form

$$\frac{dU_i^A}{dt} = -2\bar{W}_{AB}U_i^A(t) + \bar{W}_{BA}[U_i^B(t) + U_{i-1}^B(t)], \quad (4)$$

$$\frac{dU_i^B}{dt} = -2\bar{W}_{BA}U_i^B(t) + \bar{W}_{AB}[U_i^A(t) + U_{i+1}^A(t)], \quad (5)$$

where \bar{W}_{AB} and \bar{W}_{BA} are effective transition rates which are given by

$$\bar{W}_{AB} = W_{AB}(1 - \langle P_B \rangle) + W_{BA}\langle P_B \rangle, \quad (6)$$

$$\bar{W}_{BA} = W_{BA}(1 - \langle P_A \rangle) + W_{AB}\langle P_A \rangle. \quad (7)$$

A general solution to Eqs. (4) and (5) can be ob-

tained by taking the Laplace transform with respect to the time variable and Fourier transforms with respect to the sublattice sites. We define

$$\tilde{U}_A(k, s) = \sum_{n_A} e^{-ikr_{n_A}} \int_0^\infty dt e^{-st} U_{n_A}^A(t), \quad (8)$$

$$\tilde{U}_B(k, s) = \sum_{n_B} e^{-ikr_{n_B}} \int_0^\infty dt e^{-st} U_{n_B}^B(t), \quad (9)$$

where r_{n_A} and r_{n_B} denote the positions of the sites on the A and B sublattices, respectively. From (4) and (5) we obtained the coupled equations

$$s\tilde{U}_A(k, s) - U_0^A(k) = -2\overline{W}_{AB}\tilde{U}_A(k, s) + 2\overline{W}_{BA}\cos(ka)\tilde{U}_B(k, s), \quad (10)$$

$$s\tilde{U}_B(k, s) - U_0^B(k) = -2\overline{W}_{BA}\tilde{U}_B(k, s) + 2\overline{W}_{AB}\cos(ka)\tilde{U}_A(k, s), \quad (11)$$

where a is the lattice constant and $U_0^A(k)$ and $U_0^B(k)$ are the Fourier transforms of the initial values $U_{n_A}^A(0)$ and $U_{n_B}^B(0)$. Upon inverting the solution to (10) and (11) we obtain the results

$$U_{n_A}^A(t) = \frac{a}{\pi} \int_{-\pi/2a}^{\pi/2a} dk \frac{\cos(kr_{n_A})}{s_+(k) - s_-(k)} \left\{ 2\overline{W}_{BA} [U_0^A(k) + \cos(ka)U_0^B(k)] \times (e^{-s_-(k)t} - e^{-s_+(k)t}) + U_0^A(k) [s_+(k)e^{-s_+(k)t} - s_-(k)e^{-s_-(k)t}] \right\}, \quad (12)$$

$$U_{n_B}^B(t) = \frac{a}{\pi} \int_{-\pi/2a}^{\pi/2a} dk \frac{\cos(kr_{n_B})}{s_+(k) - s_-(k)} \left\{ 2\overline{W}_{AB} [U_0^B(k) + \cos(ka)U_0^A(k)] \times (e^{-s_-(k)t} - e^{-s_+(k)t}) + U_0^B(k) [s_+(k)e^{-s_+(k)t} - s_-(k)e^{-s_-(k)t}] \right\}, \quad (13)$$

where

$$s_{\pm}(k) = \overline{W}_{AB} + \overline{W}_{BA} \pm [(\overline{W}_{AB} - \overline{W}_{BA})^2 + 4\overline{W}_{AB}\overline{W}_{BA}\cos^2(ka)]^{1/2}, \quad (14)$$

and we have made use of the assumption that $N \gg 1$ in order to replace the sums over k by equivalent integrals. Equations (12) and (13), it should be noted, are the exact solutions for the single particle problem.

III. SPECIAL CASES

In this section we consider two limiting cases of the general model. In the first of these we take $W_{AB} = W_{BA} = W$. In this limit the nonlinear terms in Eqs. (1) and (2) drop out resulting in the equation

$$\frac{dP_i(t)}{dt} = -2WP_i(t) + W[P_{i+1}(t) + P_{i-1}(t)], \quad (15)$$

where we no longer distinguish between the two sublattices in the definition of $P_i(t)$. Since (15) is a linear equation we can express the solutions of the many particle problem as linear combinations of the solution to the problem of the kinetics of a single particle. The latter are given by^{5,7}

$$P_i(t) = e^{-2Wt} I_{|i-k|}(2Wt), \quad (16)$$

corresponding to the initial condition $P_i(0) = \delta_{ik}$.

Here $I_n(z)$ denotes the modified Bessel function of order n .

In analyzing the dynamics it is convenient to introduce the conditional probability $\langle P(t) \rangle$ defined by

$$\langle P(t) \rangle = \lim_{N \rightarrow \infty} \sum_{i=1}^N \frac{P_i(0)P_i(t)}{NC}, \quad (17)$$

where C is the concentration of particles. The function $\langle P(t) \rangle$ is the probability that a site which is occupied at $t=0$ is also occupied at time t . It has the asymptotic behavior

$$\lim_{t \rightarrow \infty} \langle P(t) \rangle = C. \quad (18)$$

Because of the linear nature of the solutions we can express $\langle P(t) \rangle$ for random initial conditions in the form

$$\langle P(t) \rangle = e^{-2Wt} I_0(2Wt) + 2Ce^{-2Wt} \sum_{n=1}^{\infty} I_n(2Wt), \quad (19)$$

where the first term is the single particle or "self"-contribution and the remaining terms are the contributions from the other sites each of which has a probability C of being occupied at $t=0$.

As a result of the identity⁸

$$e^z = I_0(z) + 2 \sum_{n=1}^{\infty} I_n(z), \quad (20)$$

Eq. (19) reduces to⁹

$$P(t) = (1 - C)e^{-2Wt} I_0(2Wt) + C, \quad (21)$$

which has the limiting behavior

$$P(t) \sim C + (1 - C)/(4\pi Wt)^{1/2}, \quad (22)$$

$$P(t) \sim 1 - 2Wt(1 - C) \quad (23)$$

for long and short times, respectively.

The second limit arises in a situation where the number of particles is equal to one-half the number of sites so that $\langle P_A \rangle + \langle P_B \rangle = 1$. In this limit the linearized rate equations reduce to the form

$$\frac{dU_i^A(t)}{dt} = -2\bar{W}U_i^A(t) + \bar{W}[U_i^B(t) + U_{i-1}^B(t)], \quad (24)$$

$$\frac{dU_i^B(t)}{dt} = -2\bar{W}U_i^B(t) + \bar{W}[U_i^A(t) + U_{i+1}^A(t)], \quad (25)$$

where \bar{W} is an average transition rate defined by

$$\bar{W} = W_{AB}\langle P_A \rangle + W_{BA}\langle P_B \rangle. \quad (26)$$

Thus when $\langle P_A \rangle + \langle P_B \rangle = 1$ the sublattices have the same effective transition rate in the linear regime. As shown in the Appendix the parameter \bar{W} also enters in the formal solution to the general problem.

We can exploit the similarity between Eqs. (24) and (25) and Eq. (15) to develop approximate expressions for the sublattice conditional probabilities, $\langle P_A(t) \rangle$, and $\langle P_B(t) \rangle$, which are defined by

$$\langle P_A(t) \rangle = \lim_{N \rightarrow \infty} \sum_{n_A} P_{n_A}(0) P_{n_A}(t) / {}_{1/2}^N \langle P_A \rangle, \quad (27)$$

$$\langle P_B(t) \rangle = \lim_{N \rightarrow \infty} \sum_{n_B} P_{n_B}(0) P_{n_B}(t) / {}_{1/2}^N \langle P_B \rangle, \quad (28)$$

with the limiting values

$$\langle P_A(0) \rangle = \langle P_B(0) \rangle = 1, \quad (29)$$

$$\langle P_A(\infty) \rangle = \langle P_A \rangle, \quad (30)$$

$$\langle P_B(\infty) \rangle = \langle P_B \rangle. \quad (31)$$

Assuming initial conditions corresponding to an equilibrium distribution of particles we can approximate $\langle P_A(t) \rangle$ and $\langle P_B(t) \rangle$ by expressions of the form

$$\alpha_1 \left(e^{-2\bar{W}t} I_0(2\bar{W}t) + 2 \sum_{n=1}^{\infty} C_n^0 e^{-2\bar{W}t} I_n(2\bar{W}t) \right) + \alpha_2$$

where C_n^0 is the probability that the n th site (relative to the origin) is occupied at $t=0$ and α_1 and α_2 are constants. With α_1 and α_2 chosen to give the correct initial and asymptotic values we have, for the approximate functions,

$$\begin{aligned} \langle P_A(t) \rangle_{APP} = & 2(1 - \langle P_A \rangle)^2 e^{-2\bar{W}t} I_0(2\bar{W}t) \\ & + (1 - \langle P_A \rangle)(2\langle P_A \rangle - 1) e^{-4\bar{W}t} + \langle P_A \rangle, \end{aligned} \quad (32)$$

$$\begin{aligned} \langle P_B(t) \rangle_{APP} = & 2(1 - \langle P_B \rangle)^2 e^{-2\bar{W}t} I_0(2\bar{W}t) \\ & + (1 - \langle P_B \rangle)(2\langle P_B \rangle - 1) e^{-4\bar{W}t} + \langle P_B \rangle, \end{aligned} \quad (33)$$

where in obtaining (32) and (33) we have made use of the identities⁸

$$\cosh z = I_0(z) + 2 \sum_{n=1}^{\infty} I_{2n}(z), \quad (34)$$

$$\sinh z = 2 \sum_{n=0}^{\infty} I_{2n+1}(z). \quad (35)$$

For $W_{BA} = W_{AB}$, Eqs. (28) and (29) agree with the exact answer given by Eq. (21). An indication of their accuracy for $W_{BA}/W_{AB} = 10$ ($\langle P_A \rangle = 0.76$, $\langle P_B \rangle = 0.24$) is provided by Figs. 1 and 2 where we have compared (32) and (33) with the results obtained by integrating the nonlinear rate equations for a lattice of 1000 sites. The numerical output was averaged over 40 initial configurations each with 380 particles distributed at random on the A sites and 120 particles distributed at random on the B sites.

The approximate theory is accurate at large times. However, the initial slopes are not given correctly since

$$\frac{d\langle P_A(0) \rangle}{dt} = -2W_{AB}(1 - \langle P_B \rangle), \quad (36)$$

whereas

$$\begin{aligned} \frac{d\langle P_A(0) \rangle}{dt}_{APP} = & -4\bar{W}[(1 - \langle P_A \rangle)^2 \\ & + (1 - \langle P_A \rangle)(2\langle P_A \rangle - 1)], \end{aligned} \quad (37)$$

with corresponding results for $d\langle P_B(0) \rangle/dt$.

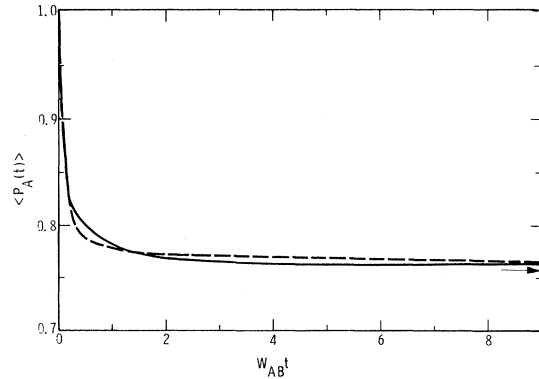


FIG. 1. $\langle P_A(t) \rangle$ vs $W_{AB}t$ for $W_{BA}/W_{AB} = 10$ and $\langle P_A \rangle + \langle P_B \rangle = 1$. The solid curve is obtained by numerical integration of Eqs. (1) and (2). The broken curve is the linear approximation given by Eq. (32). The arrow indicates the asymptote.

Nevertheless, both curves exhibit the same qualitative features, namely, a rapid initial decay followed by a slow approach to the asymptote.

IV. DISCUSSION

Upon comparing what is obtained by evaluating Eq. (21) with the curves in Figs. 1 and 2 it becomes evident that the presence of the nonlinear terms in the rate equations for $W_{AB} \neq W_{BA}$ does not have a qualitative effect on the conditional probabilities other than to alter their asymptotic values. This does not necessarily hold for other dynamical functions, however. For example, one function of interest in transport problems is the current-current correlation function $\langle J(t)J(0) \rangle$. As we will show the particle current $J(t)$ and hence $\langle J(t)J(0) \rangle$ change qualitatively when the two sublattices become equivalent.

We can obtain an expression for J by making use of the continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0, \quad (38)$$

where n is the particle density and j is the current density. In the lattice analog of (38) we associate P_i with n . The counterpart of $\partial j/\partial x$ is obtained from the rate equations. In the case of equal transition rates we have [cf. Eq. (15)]

$$\frac{dP_i}{dt} + [W(P_i - P_{i+1}) - W(P_{i-1} - P_i)] = 0. \quad (39)$$

Comparing (39) with (39) we identify the discrete current density

$$j_i = aW(P_i - P_{i-1}). \quad (40)$$

The total current is then given by

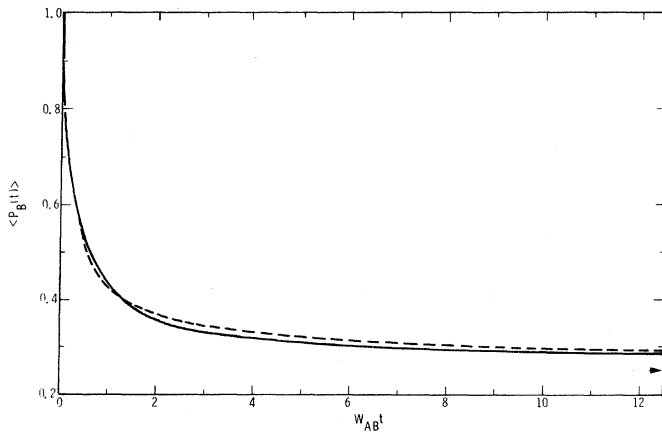


FIG. 2. $\langle P_B(t) \rangle$ vs $W_{AB}t$ for $W_{BA}/W_{AB} = 10$ and $\langle P_A \rangle + \langle P_B \rangle = 1$. The solid curve is obtained by numerical integration of Eqs. (1) and (2). The broken curve is the linear approximation given by Eq. (33). The arrow indicates the asymptote.

$$J = \sum_i j_i = aW \sum_i (P_i - P_{i+1}). \quad (41)$$

From (40) and (41) it is evident that j_i is essentially equivalent to $-a^2 W \partial n / \partial x$ (Fick's law), and hence J depends only on the densities at the beginning and end of the chain. This feature is a consequence of the absence of nonlinear correlation terms in the rate equations.

When $W_{AB} \neq W_{BA}$ a similar analysis leads to an expression for the current of the form

$$J = a(W_{AB} - W_{BA}) \sum_i P_i^A (P_{i-1}^B - P_i^B) + \dots, \quad (42)$$

where the dots represent boundary terms. In the limit of large N we can neglect the contribution from the boundary terms and write $\langle J(t)J(0) \rangle$ in the form

$$\begin{aligned} \langle J(t)J(0) \rangle &= a^2 (W_{AB} - W_{BA})^2 \\ &\times \sum_{i,j} \langle P_i^A(t) [P_{i-1}^B(t) - P_i^B(t)] \\ &\times P_j^A(0) [P_{j-1}^B(0) - P_j^B(0)] \rangle, \end{aligned} \quad (43)$$

where the brackets are interpreted as referring to a solution of the rate equations with initial conditions corresponding to an equilibrium distribution of particles. The presence of the four-particle correlations in (43) is a characteristic feature of the inequivalent sublattice model and leads to an expression for $\langle J(t)J(0) \rangle$ which is independent of the boundaries of the chain, in contrast to the results obtained with Eq. (41).

In analyzing $\langle J(t)J(0) \rangle$ it is convenient to intro-

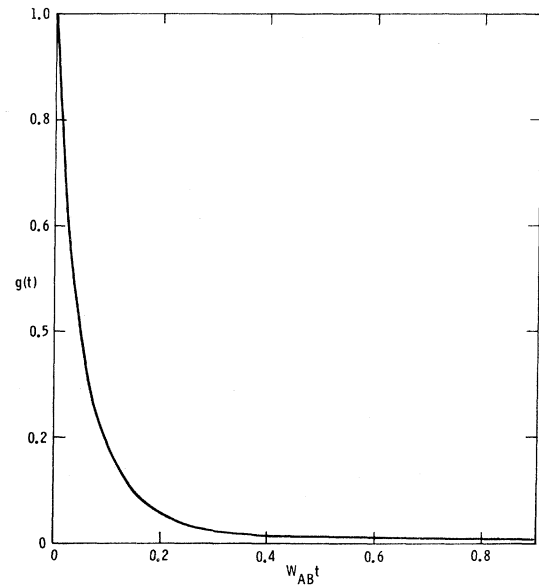


FIG. 3. Normalized current-current correlation function $g(t)$ vs $W_{AB}t$ for $W_{BA}/W_{AB} = 10$ and $\langle P_A \rangle + \langle P_B \rangle = 1$.

duce the normalized correlation junction $g(t) = \langle J(t)J(0) \rangle / \langle J(0)J(0) \rangle$, where $\langle J(0)J(0) \rangle$ is given by

$$\begin{aligned} \langle J(0)J(0) \rangle &= a^2(W_{AB} - W_{BA})^2 N \langle P_A \rangle \\ &\times (1 - \langle P_A \rangle) \langle P_B \rangle (1 - \langle P_B \rangle). \end{aligned} \quad (44)$$

Our results for $g(t)$ are shown in Fig. 3. The curve is obtained by averaging $\langle J(t)J(0) \rangle$ over forty runs on a lattice with 1000 sites. As in Figs. 1 and 2 it is assumed that $W_{BA}/W_{AB} = 10$. In contrast to the conditional probabilities the current-current correlation function approaches its asymptotic value extremely rapidly. Since the conditional probabilities are essentially density-density correlation functions the difference arises in the slow, diffusive ($\sim t^{-1/2}$) decay of the small-amplitude long-wavelength fluctuations in the particle density, an effect which is not present in the relaxation of the fluctuations of the current.

ACKNOWLEDGMENTS

We would like to thank Dr. P. M. Richards for stimulating our interest in this problem and Dr. W. J. Camp for bringing Ref. 6 to our attention.

APPENDIX

In this Appendix we outline an analysis of the inequivalent sublattice model using the spin-operator formalism of Ref. 6. In the interests of simplicity we consider only the case of the half-filled band. In order to make contact with the operator formalism we identify $P_i^{A,B}$ with $\frac{1}{2}(1 + \sigma_{n_A, n_B}^z)$ where σ^z is the Pauli operator with eigenvalues ± 1 . The density operator characterizing the equilibrium distribution is given by

$$\rho_{\text{eq}} = \exp\left(\sum_{n_A} \sigma_{n_A}^z - \sum_{n_B} \sigma_{n_B}^z\right), \quad (A1)$$

where the parameter h is related to $\langle P_A \rangle$ through the equation

$$\begin{aligned} \langle P_A \rangle &= \frac{1}{2}(1 + \langle \sigma_{n_A}^z \rangle) = \frac{1}{2}(1 + \tanh h) \\ &= 1 - \langle P_B \rangle. \end{aligned} \quad (A2)$$

The probability distribution is represented by a state vector $|P(t)\rangle$, whose time dependence is determined by the master equation

$$\frac{d}{dt} |P(t)\rangle = \mathfrak{B} |P(t)\rangle, \quad (A3)$$

where \mathfrak{B} is the master operator. The expectation value of any observable X at time t is given by

$$\langle X \rangle_t = \langle \mathbf{1} | X | P(t) \rangle, \quad (A4)$$

where $|\mathbf{1}\rangle$ denotes the unit state with the spinor

representation

$$|\mathbf{1}\rangle = \binom{1}{1}_1 \times \binom{1}{1}_2 \times \cdots \times \binom{1}{1}_N. \quad (A5)$$

The master operator corresponding to Eqs. (1) and (2) can be written

$$\begin{aligned} \mathfrak{B} &= W_{AB} \sum_{n \text{ odd}} \sigma_n^- (\sigma_{n+1}^+ + \sigma_{n-1}^+) \\ &+ W_{BA} \sum_{n \text{ even}} \sigma_n^- (\sigma_{n+1}^+ + \sigma_{n-1}^+) \\ &- (W_{AB} + W_{BA})N, \end{aligned} \quad (A6)$$

where we have identified the odd values of n with the A sites and the even values of n with the B sites. The symbols σ^\pm denote the raising and lowering operators $\frac{1}{2}(\sigma^x \pm i\sigma^y)$.

For values of W_{AB} and W_{BA} consistent with the detailed balance relation we can symmetrize the master operator by means of the similarity transformation⁶

$$\hat{\mathfrak{B}} = \rho_{\text{eq}}^{-1/2} \mathfrak{B} \rho_{\text{eq}}^{1/2}. \quad (A7)$$

We have

$$\rho_{\text{eq}}^{-1/2} \sigma_n^+ \rho_{\text{eq}}^{1/2} = \sigma_n^+ \begin{cases} e^{-h}, & n \text{ odd}, \\ e^h, & n \text{ even}; \end{cases} \quad (A8)$$

$$\rho_{\text{eq}}^{-1/2} \sigma_n^- \rho_{\text{eq}}^{1/2} = \sigma_n^- \begin{cases} e^h, & n \text{ odd}, \\ e^{-h}, & n \text{ even}, \end{cases} \quad (A9)$$

so that

$$\hat{\mathfrak{B}} = \hat{W} \sum_n (\sigma_n^- \sigma_{n+1}^+ + \sigma_n^+ \sigma_{n+1}^-) - (W_{AB} + W_{BA})N, \quad (A10)$$

where

$$\begin{aligned} \hat{W} &= W_{AB} e^{2h} = W_{BA} e^{-2h} \\ &= W_{AB} \langle P_A \rangle + W_{BA} \langle P_B \rangle, \end{aligned} \quad (A11)$$

the last equations following from (A2) and the detailed balance relation, Eq. (3). Note that \hat{W} is equal to the average relaxation rate \bar{W} in Eqs. (24) and (25).

The operator $\hat{\mathfrak{B}}$ is identical in form to the Hamiltonian of the XY model^{10,11} and is readily diagonalized in terms of the Fermi operators ξ_q, ξ_q^\dagger ($\{\xi_q, \xi_{q'}^\dagger\} = \delta_{q,q'}, -\pi/a \leq q \leq \pi/a$):

$$\hat{W} = 2\hat{W} \sum_q \cos(qa) \xi_q^\dagger \xi_q + \text{const.} \quad (A12)$$

Although the master operator can be diagonalized the calculation of the expectation values is made complicated by the condition that the similarity transformation also be applied to the state vectors, i.e.,

$$\langle X \rangle_t = \langle \mathbf{0} | X | \psi(t) \rangle, \quad (A13)$$

where we have $|0\rangle = \rho_{\mathbf{q}}^{1/2} |1\rangle$ and the vector $|\psi(t)\rangle = \rho_{\mathbf{q}}^{-1/2} |P(t)\rangle$ is a solution of

$$\frac{d}{dt} |\psi(t)\rangle = \mathbb{B} |\psi(t)\rangle. \quad (\text{A14})$$

The difficulty arises because $\rho_{\mathbf{q}}$ in the fermion representation has the form

$$\rho_{\mathbf{q}} = \exp\left(2h \sum_{\mathbf{q}} \xi_{\mathbf{q}}^{\dagger} \xi_{\mathbf{q}+\pi/a}\right). \quad (\text{A15})$$

The bilinear combination $\xi_{\mathbf{q}}^{\dagger} \xi_{\mathbf{q}+\pi/a}$ in the exponential leads to complicated expressions for the expectation values which we have not been able to simplify except in the trivial case $h=0$. In this limit we make contact with the theory of Sec. III through the integral representation⁸

$$I_n(z) = \frac{a}{\pi} \int_0^{\pi/a} e^{z \cos(qa)} \cos(nqa) dq. \quad (\text{A16})$$

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