

Stochastic dynamics of diffusive deposition-evaporation processes in the presence of defects

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An exact calculation of the autocorrelation function is presented for the dimer deposition-evaporation model with single particle diffusion in the presence of a bond defect. Different time regimes are separated by crossover times, which are determined by the interplay between the spatial and temporal characteristics of the autocorrelation function. For certain choices of the stochastic rates, localized defect modes can alter the ultimate long-time exponential decay rate of the entire system.

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I. INTRODUCTION

Stochastic models of various kinds [1,2] have recently attracted a great deal of attention. Most of the models so far investigated are perfectly pure systems, which possess translational symmetry. However, in any real physical application, such as surface or interface growth or chemical reactions on surfaces, impurities or defects are unavoidable. It is our aim here to start to examine the effect of defects on stochastic processes and to gain some insight into the stochastic behavior of disordered systems.

Among the pure stochastic systems currently studied are stochastic particle hopping models [3], growth models [4,5], and deposition-evaporation models [6]. For particular stochastic hopping processes the effect of a single defect has been recently studied numerically [7] and analytically [8]. In this paper we treat an impure deposition-evaporation model which also includes particle hopping.

Specifically, we present an exact calculation of the autocorrelation function for the dimer deposition-evaporation models with single particle diffusion in the presence of a bond defect, over which both the deposition-evaporation rate and the diffusive hopping rate can be different from those for the rest of the system. It turns out that this single defect bond can in general support two localized bound states. With certain choices of the stochastic rates, these bound states correspond to defect modes which are below the bulk energy band and hence change the intrinsic long-time behavior of the entire system.

II. MASTER EQUATION AND XXZ SPIN CHAIN

We consider a one-dimensional (1D) lattice on which the elementary stochastic processes are deposition and evaporation of dimers with the same rate ϵ and hop-

ping of single particles to either one of the two nearest neighbor sites with equal probability h . Since we only consider the case of single occupancy, the deposition process can only occur when the two chosen neighboring sites are empty or the evaporation when the two sites are occupied. The hopping process can take place only if the two chosen sites have one site occupied and the other empty. Due to this mutual exclusion, at any given time (or updating step) t , only one of the four above-mentioned processes can be attempted at any randomly chosen neighboring-site pair.

The dynamics of this stochastic system can be described by the master equation, which governs the time evolution of the probability $P(s, t)$ of finding the system in a certain particle configuration $|s\rangle$ at time t . If $W(s \rightarrow s')$ denotes the rate or transition probability per unit time at which configuration $|s\rangle$ evolves to $|s'\rangle$, the master equation is

$$\frac{\partial}{\partial t} P(s, t) = \sum_{s'} [W(s' \rightarrow s) P(s', t) - W(s \rightarrow s') P(s, t)]. \quad (1)$$

The basis vectors $\{|s\rangle\}$ form a complete orthonormal set. The ensemble averaged state vector for the system at time t can then be defined by

$$|P(t)\rangle = \sum_s P(s, t) |s\rangle. \quad (2)$$

It is easy to check that the master equation (1) can now be rewritten as

$$\frac{\partial}{\partial t} |P(t)\rangle = -H |P(t)\rangle, \quad (3)$$

where the transition operator H is defined in terms of its matrix elements:

$$\langle s' | H | s \rangle = -W(s \rightarrow s'), \quad s' \neq s \quad (4)$$

$$\langle s | H | s \rangle = \sum_{s' \neq s} W(s \rightarrow s').$$

From Eq. (3) it is clear that the steady state of the system corresponds to the ground state of the transition operator

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H with zero eigenvalue $E_0 = 0$. Any eigenvalues with positive real part E correspond to decaying states with lifetime $1/E$. It is also worthwhile to note that every column of matrix H adds up to zero due to probability conservation.

It is again convenient to use the analogy between the present system and quantum spin- $\frac{1}{2}$ models. Using the spinors $\alpha(n)$ or $\beta(n)$ to denote a particle or a vacancy at site n , the four elementary processes of the stochastic system under consideration can be described by

$$\sigma_n^+ \sigma_{n+1}^+ \beta(n) \beta(n+1) = \alpha(n) \alpha(n+1) \quad (\text{with deposition rate } \varepsilon),$$

$$\sigma_n^- \sigma_{n+1}^- \alpha(n) \alpha(n+1) = \beta(n) \beta(n+1) \quad (\text{with evaporation rate } \varepsilon),$$

$$\sigma_n^- \sigma_{n+1}^+ \alpha(n) \beta(n+1) = \beta(n) \alpha(n+1) \quad (\text{with right hopping rate } h),$$

$$\sigma_n^+ \sigma_{n+1}^- \beta(n) \alpha(n+1) = \alpha(n) \beta(n+1) \quad (\text{with left hopping rate } h).$$

Therefore, the off-diagonal part of the transition operator, which only connects two different state vectors $|s\rangle$ and $|s'\rangle$ through a single elementary process listed above, should take the form

$$\begin{aligned} & \sum_{s,s'} |s'\rangle \langle s'| H |s\rangle \langle s| \\ &= -\varepsilon \sum_n (\sigma_n^+ \sigma_{n+1}^+ + \sigma_n^- \sigma_{n+1}^-) \\ & \quad - h \sum_n (\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+) \\ &= \frac{1}{2} \sum_n [-(\varepsilon + h) \sigma_n^x \sigma_{n+1}^x + (\varepsilon - h) \sigma_n^y \sigma_{n+1}^y], \end{aligned} \quad (5)$$

where the prime denotes the exclusion of $s = s'$ terms and $\sigma_n^\pm = (\sigma_n^x \pm i\sigma_n^y)/2$. From Eq. (4) it is clear that the diagonal part of the transition operator H counts the total number of ways in which a configuration $|s\rangle$ can evolve to different ones $|s'\rangle$ through a single elementary process. In terms of the occupation number operator at site m , $n_m \equiv \sigma_m^+ \sigma_m^- = (1 + \sigma_m^z)/2$, we can write the diagonal part of the transition operator as

$$\begin{aligned} & \sum_s |s\rangle \langle s| H |s\rangle \langle s| \\ &= \varepsilon \sum_m [(1 - n_m)(1 - n_{m+1}) + n_m n_{m+1}] \\ & \quad + h \sum_m [n_m (1 - n_{m+1}) + (1 - n_m) n_{m+1}] \\ &= \frac{1}{2} \sum_n [2h + (\varepsilon - h)(1 + \sigma_n^z \sigma_{n+1}^z)]. \end{aligned} \quad (6)$$

It is then easy to see that the total transition operator H , obtained by combining (5) and (6), can always be mapped into the ‘‘Hamiltonian’’ of the XXZ spin- $\frac{1}{2}$ chain. For example, for the case of $\varepsilon > h$, we can introduce the following sublattice rotations:

$$(\sigma_{2n}^x, \sigma_{2n}^y, \sigma_{2n}^z) = (-\tau_{2n}^z, \tau_{2n}^y, \tau_{2n}^x), \quad (7)$$

$$(\sigma_{2n+1}^x, \sigma_{2n+1}^y, \sigma_{2n+1}^z) = (-\tau_{2n+1}^z, -\tau_{2n+1}^y, -\tau_{2n+1}^x),$$

which leads to

$$\begin{aligned} H = & -\frac{1}{2}(\varepsilon - h) \sum_n [\tau_n^x \tau_{n+1}^x + \tau_n^y \tau_{n+1}^y \\ & + (1 + \Delta) \tau_n^z \tau_{n+1}^z], \end{aligned} \quad (8)$$

where $\Delta \equiv 2h/(\varepsilon - h) > 0$. Hence the ground states are the two ferromagnetically aligned configurations: $|F\rangle_+$ with all spins up and $|F\rangle_-$ with all spins down in the τ representation.

III. STEADY STATES AND THE AUTOCORRELATION FUNCTION

Since any physical state must have definite parity (with either even or odd number of particles in the original particle or σ representation), it can be shown [9] that the two physical and normalized steady states are the linear combinations of the above two configurations:

$$|S_\pm\rangle = \frac{\sqrt{2}}{2} (|F\rangle_+ \pm |F\rangle_-) \quad (9)$$

for systems with even (upper sign) or odd (lower sign) number of particles. Here and in the rest of this paper, any state in Dirac’s bra-ket notation are understood to be in the τ representation.

The main purpose of this paper is to study the long time behavior of the autocorrelation function in the presence of isolated defects. The autocorrelation function is defined by

$$\begin{aligned} C_{n,m}(t) \equiv & \langle S | n_n e^{-Ht} n_m | S \rangle \\ & - \langle S | n_n | S \rangle \langle S | n_m | S \rangle, \end{aligned} \quad (10)$$

where the steady state $|S\rangle$ is either of the two states in (9), depending on the parity of the system’s initial configuration. The particle number operator at a given site m can be rewritten in terms of τ operators: $n_m = (1 + \sigma_m^z)/2 = (1 + \tau_m^x)/2 = (1 \pm \tau_m^+ \pm \tau_m^-)/2$ for m being an even (upper sign) or an odd (lower sign) integer. This gives immediately

$$n_m |S_\pm\rangle = \frac{1}{2} |S\rangle + (-1)^m \frac{\sqrt{2}}{4} (|m\rangle_+ \pm |m\rangle_-), \quad (11)$$

where $|m\rangle_+$ denotes the state with a single spin flipped at site m in the otherwise all-spin-up background and $|m\rangle_-$ that in the all-spin-down background. Using (8) it is also easy to check the following relation:

$$H|n\rangle_{\pm} = 2(\varepsilon + h)|n\rangle_{\pm} - (\varepsilon - h)(|n + 1\rangle_{\pm} + |n - 1\rangle_{\pm}), \quad (12)$$

which means that an operation of H (or function of H) on a single-spin-flipped state will only produce a single-spin-flipped state(s). This enables us to obtain readily, from (10) and (11),

$$C_{n,m}(t) = \frac{1}{4}(-1)^{n+m} \langle n|e^{-Ht}|m\rangle, \quad (13)$$

where the state $|n\rangle$ can be either one of the two introduced in (11) and the above expression is also independent of the choice between $|S_+\rangle$ and $|S_-\rangle$.

IV. GREEN'S FUNCTION AND DEFECT MODES

For a system with translational invariance as described in (8) and (12), the autocorrelation function (10) can be calculated analytically by Fourier transformation. However, in the presence of defects, it is convenient to make use of the two-point Green's function, which is defined as

$$G_{n,m}(E) \equiv \langle n|(E - H)^{-1}|m\rangle. \quad (14)$$

The relation between the Green's function and the autocorrelation function can be derived by inserting the complete orthonormal set of eigenstates of H into (14) and using the well-known relation $\text{Im} 1/(x - i0^+) = \pi \delta(x)$. It is then not difficult to find that

$$C_{n,m}(t) = \frac{(-1)^{n+m}}{4\pi} \text{Im} \int_{-\infty}^{\infty} G_{n,m}(E - i0^+) e^{-Et} dE. \quad (15)$$

We now proceed to calculate the Green's function of the system with a bond defect situated between, say, site 0 and site 1. The site defect case is also interesting in other contexts, but is not physically relevant for the present dimer model. If we use ε^* and h^* to denote the deposition-evaporation rate and the hopping rate over the defect bond, the Hamiltonian equation (12) is then modified to

$$H|n\rangle = 2(\varepsilon + h)|n\rangle - (\varepsilon - h)(|n + 1\rangle + |n - 1\rangle) + \delta_{n,0}(\varepsilon - h)(u|n\rangle - v|n + 1\rangle) + \delta_{n,1}(\varepsilon - h)(u|n\rangle - v|n - 1\rangle), \quad (16)$$

where $u \equiv (\varepsilon^* - \varepsilon + h^* - h)/(\varepsilon - h)$ and $v \equiv (\varepsilon^* - \varepsilon - h^* + h)/(\varepsilon - h)$. It is then clear that the matrix $\mathbf{H} - E\mathbf{I}$ in the single-spin-flipped-state representation can be written as a tridiagonal matrix \mathbf{T} , whose inverse is known, plus a perturbing matrix \mathbf{V} , whose only nonvanishing part is a 2×2 submatrix along the main diagonal. From (14) we obtain formally

$$\mathbf{G}(E) = -(\mathbf{T} + \mathbf{V})^{-1} = -(\mathbf{I} + \mathbf{T}^{-1}\mathbf{V})^{-1}\mathbf{T}^{-1}, \quad (17)$$

where \mathbf{I} is the unit matrix. Since the inverse of $(\mathbf{I} +$

$\mathbf{T}^{-1}\mathbf{V})$ can also be analytically obtained (see Appendix A), we finally have, for both n and $m \geq 1$,

$$(\varepsilon - h)G_{n,m}(E) = \frac{x^{|n-m|}}{x - x^{-1}} - \frac{x^{n+m}}{x - x^{-1}} \frac{x_1 x_2 f(x)}{(x - x_1)(x - x_2)}; \quad (18)$$

and for $n \geq 1$ and $m \leq 0$,

$$(\varepsilon - h)G_{n,m}(E) = -\frac{x^{n-m-1} x_1 x_2 (1 + v)}{(x - x_1)(x - x_2)}, \quad (19)$$

where both x_1 and x_2 are real (given below), and

$$f(x) \equiv u(x + x^{-1}) - 2v + (u + v)(u - v). \quad (20)$$

The complex x is subject to the normalizability condition $|x| \leq 1$ and is related to the energy E through the equation

$$x + x^{-1} = [2(\varepsilon + h) - E]/(\varepsilon - h). \quad (21)$$

The continuous bulk energy band corresponds to $|x| = 1$, with the lower and upper band edges at $E_b = 4h$ ($x = 1$) and $E_u = 4\varepsilon$ ($x = -1$). The localized energy modes are determined by the two factors in the Green's function denominators in (18) and (19). In the first factor ($x - x_1$), which turns out to be independent of h^* , we have

$$x_1 = 1 - 2(h - \varepsilon^*)(\varepsilon + h - 2\varepsilon^*)^{-1}, \quad (22)$$

$$E_1 = E_b - 4(h - \varepsilon^*)^2 (\varepsilon + h - 2\varepsilon^*)^{-1}. \quad (23)$$

From the above two equations, it is easy to see that in order to satisfy both the localization condition $|x| < 1$ and to have the mode below the bulk band $E_b > E_1$, which will dominate the long-time behavior of the autocorrelation, we need to have $\varepsilon^* < h$. Similarly, in the second factor ($x - x_2$), which is independent of ε^* , we have

$$x_2 = 1 - 2(h - h^*)(\varepsilon + h - 2h^*)^{-1}, \quad (24)$$

$$E_2 = E_b - 4(h - h^*)^2 (\varepsilon + h - 2h^*)^{-1}. \quad (25)$$

This means that the second bound state can be formed below the bulk band if $h^* < h$.

Note that since the spin chain should have ferromagnetic coupling on every single bond in order to have stable ferromagnetic ground states (and hence well-defined steady states), we shall also require that $\varepsilon^* > h^*$. Therefore, in order to have two localized states associated with the defect below the bulk band, we have to have the following rate ordering:

$$\varepsilon > h > \varepsilon^* > h^*, \quad (26)$$

which then leads to

$$x_1 - x_2 = \frac{2(\varepsilon^* - h)(\varepsilon - h)}{(\varepsilon + h - 2h^*)(\varepsilon + h - 2\varepsilon^*)} > 0, \quad (27)$$

$$E_1 - E_2 = 4(\varepsilon^* - h^*) \times \frac{(\varepsilon - h^*)(h - \varepsilon^*) + (\varepsilon - \varepsilon^*)(h - h^*)}{(\varepsilon + h - 2h^*)(\varepsilon + h - 2\varepsilon^*)} > 0. \quad (28)$$

Another point worth mentioning is that it is impossible to push any one of the defect energy modes down to zero because the condition required for having a zero-energy mode (ε^* or $h^* = \sqrt{\varepsilon h}$) cannot be simultaneously satisfied with the localization condition $|x_{1,2}| < 1$ and $E_{1,2} < E_b$ from (22)–(25).

V. LONG-TIME BEHAVIOR AND CROSSOVERS

We now use Eq. (15) and our knowledge of the Green's function to calculate the autocorrelation function in the

steady states. From the relation between E and x in (21) we realize that the integration over the energy E can be rewritten as

$$\int_{-\infty}^{\infty} dE = -(\varepsilon - h) \int_{-1}^1 dx \frac{x - x^{-1}}{x} + 2(\varepsilon - h) \int_0^{\pi} d\theta \sin \theta, \quad (29)$$

where we have changed the variable $x = e^{i\theta}$ in the last integral. The autocorrelation function given in (15) can then be obtained analytically. Some details of the calculation are given in Appendix B, and here we only quote the results. For both n and $m \geq 1$,

$$C_{n,m}(t) = \frac{(-1)^{n+m-1}}{4} e^{-2(\varepsilon+h)t} \left(I_{|n-m|}(\tau) - \frac{x_1 x_2}{x_1 - x_2} \sum_{k=1}^{\infty} (x_1^k - x_2^k) \{u[I_{n+m-k}(\tau) + I_{n+m-k-2}(\tau)] - (2v + v^2 - u^2)I_{n+m-k-1}(\tau)\} \right) + \frac{(-1)^{n+m}}{4} \frac{x_1 x_2}{x_1 - x_2} [f(x_1) x_1^{n+m-1} e^{-E_1 t} - f(x_2) x_2^{n+m-1} e^{-E_2 t}], \quad (30)$$

where the argument in the modified Bessel function $I_n(\tau)$ is defined by $\tau \equiv 2(\varepsilon - h)t$, and $f(x_i)$, x_i , and E_i are given in (20) and (22)–(25). For $n \geq 1$ and $m \leq 0$, we have

$$C_{n,m}(t) = \frac{(-1)^{n+m}}{4} \frac{x_1 x_2 (1+v)}{x_1 - x_2} \left((x_1^2 - 1) x_1^{n-m-3} e^{-E_1 t} - (x_2^2 - 1) x_2^{n-m-3} e^{-E_2 t} + e^{-2(\varepsilon+h)t} \sum_{k=1}^{\infty} (x_1^k - x_2^k) [I_{n-m-k-1}(\tau) - I_{n-m-k-3}(\tau)] \right). \quad (31)$$

If the stochastic rates satisfy the inequalities (26), the two bound state energies E_1 and E_2 are both below the lower edge of the bulk energy band $E_b = 4h$ and will in turn dominate the long time behavior of the autocorrelation functions. However, since $|x_2| < |x_1| < 1$, the exponential decay characteristics, dictated by $E_{1,2}$ ($E_1 > E_2$), will both be quenched by the spatial factors $x_{1,2}^{n \pm m}$ for earlier times before a crossover time t_1 is reached. For $t < t_1$, the autocorrelation function decays also exponentially but with a faster rate essentially identical to that for the pure system: $t^{-1/2} e^{-E_b t}$ ($E_b > E_1$). Not until a second crossover time t_2 is passed should we expect to see the intrinsic long time behavior of the autocorrelation function, which decays as $e^{-E_2 t}$. The second crossover time t_2 can be easily defined by, for both (30) and (31),

$$t_2 \equiv (|n| + |m|) \frac{\ln x_1 - \ln x_2}{E_1 - E_2}. \quad (32)$$

To determine t_1 we use the following asymptotic expansions for the modified Bessel functions:

$$I_n(\tau) \sim \frac{e^{\tau}}{\sqrt{2\pi\tau}} \left[1 - \frac{4n^2 - 1}{8\tau} + \dots \right],$$

$$e^{-2(\varepsilon+h)t} [I_{n+1}(\tau) - I_{n-1}(\tau)] \sim -n \sqrt{\frac{2}{\pi}} \tau^{-3/2} e^{-E_b t}.$$

The first crossover time t_1 can then be defined by

$$e^{-(E_b - E_1)t_1} [2(\varepsilon - h)t_1]^{-1/2} \equiv x_1^{|n|+|m|} \quad (33)$$

for the autocorrelation in (30). For that in (31), t_1 can be obtained by changing the power $-1/2$ to $-3/2$ in the definition (33). It is physically reasonable that all the crossover times depend on the total distance of the two points concerned in the autocorrelation function from the defect. $|n| + |m|$ is the characteristic length for the defect to be "felt" by both the points.

VI. DISCUSSIONS

In the preceding section we have mainly considered the case where both the defect modes lie *below* the bulk band. This is indeed the most interesting case since it offers two crossover times and hence three time regimes for the autocorrelation function, whose decay characteristics are determined by different rates in different time regimes. More importantly, the lowest defect mode determines the ultimate long-time behavior of the system. However, it is

still worthwhile to mention that it is possible, with other choices of the stochastic rates, to have one or both of the defect modes *above* the bulk band ($E_{1,2} > E_u = 4\varepsilon$). For example, we can rewrite (22) and (23) as

$$\begin{aligned} x_1 &= -1 + 2(\varepsilon^* - \varepsilon)(2\varepsilon^* - \varepsilon - h)^{-1}, \\ E_1 &= E_u + 4(\varepsilon^* - \varepsilon)^2(2\varepsilon^* - \varepsilon - h)^{-1}. \end{aligned}$$

It is easy to see that a localized mode ($|x_1| < 1$) can appear above the bulk band ($E_1 > E_u$) if $\varepsilon^* > \varepsilon$. In this case x_1 is again real but negative.

In the pure dimer model, the case of $h = 0$ corresponds to the isotropic Heisenberg limit of the XXZ chain. The pure dimer models in one and higher dimensions have recently been studied [6]. Due to the lack of an energy gap, the systems show a slow power law decay in their autocorrelation functions. With the introduction of any isolated bond defects, the only possible defect modes with finite lifetime are those *above* the bulk band and they will not alter the long-time behaviors of the system.

It might seem surprising that a single defect is capable of changing the intrinsic long-time behavior of the entire system. This is due to the fact that the system under investigation is one dimensional. The crucial difference between 1D systems and higher-dimensional ones is that, again in the Green's function language, in 1D the number of scattering channels is so limited that the number of those channels passing through the defect can no longer be considered as only a fraction of order of $1/N$ of the total (N is the total number of sites of the system).

For the corresponding defect systems in higher-dimensions, it seems difficult to generalize the tridiagonal matrix method (described in Appendix A). However, a Green's function approach in k space can be used instead, along the line used for solid state defect problems [10]. The full Green's function is given by the usual Dyson equation

$$\begin{aligned} \mathbf{G}(\mathbf{r}, \mathbf{r}'; E) &= \mathbf{G}_0(\mathbf{r} - \mathbf{r}'; E) \\ &+ \sum_{\mathbf{s}, \mathbf{s}'} \mathbf{G}_0(\mathbf{r} - \mathbf{s}; E) \mathbf{V}(\mathbf{s}, \mathbf{s}') \mathbf{G}(\mathbf{s}', \mathbf{r}'; E). \end{aligned}$$

This can be converted to a closed form for $\mathbf{G}(\mathbf{r}, \mathbf{r}'; E)$ (involving wave-vector sums), using the local character of \mathbf{V} and the fact that $\mathbf{G}_0(\mathbf{r} - \mathbf{r}'; E)$ is diagonal in k space. Although the resulting exact expression for the full Green's function is rather difficult to reduce further, the localized mode energies E_1 and E_2 can be calculated as its isolated poles and are determined by

$$\begin{aligned} \frac{1}{h^* - h} &= \frac{2}{N} \sum_{\mathbf{k}} \frac{1 + \cos k_1}{E_1 - E(\mathbf{k})}, \\ \frac{1}{\varepsilon^* - \varepsilon} &= \frac{2}{N} \sum_{\mathbf{k}} \frac{1 - \cos k_1}{E_2 - E(\mathbf{k})}, \end{aligned}$$

assuming that the bond defect is situated in the k_1 direction. The dispersion relation is

$$\begin{aligned} E(\mathbf{k}) &\equiv 2(\varepsilon + h) - 2(\varepsilon - h) \sum_{i=1}^d \cos k_i \\ &\text{with } \mathbf{k} = (k_1, \dots, k_d). \end{aligned}$$

Other generalizations of the present defect problem to models with different deposition and evaporation rates and/or with different left-hopping and right-hopping rates are also interesting, but far more difficult to treat since in these cases we no longer have ferromagnetically aligned steady states in the quantum spin representation and the transition operator H is not necessarily Hermitian anymore.

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APPENDIX A

In this appendix we outline the main steps in the calculation of the Green's function (17) in the site representation with a bond defect by directly inverting the impure tridiagonal matrix $\mathbf{T} + \mathbf{V}$. Similar calculations for semi-infinite systems with a site defect is also available [11]. Since the matrix $\mathbf{T} \equiv \mathbf{H}_0 - E\mathbf{I}$ is for the pure system, which is translational invariant, its inverse can be easily obtained to be

$$(\mathbf{T}^{-1})_{n,m} = -(\varepsilon - h)^{-1} \frac{x^{|n-m|}}{x - x^{-1}}, \quad (\text{A1})$$

with x given in (21). This enables us to find $\mathbf{T}^{-1}\mathbf{V}$, whose only nonvanishing elements are along the two columns at $m = 0$ and $m = 1$ due to the fact that \mathbf{V} has only four nonvanishing elements. We then partition the matrix $\mathbf{I} + \mathbf{T}^{-1}\mathbf{V}$ between the two rows at $n = 0$ and 1, and the two columns at $m = 0$ and 1, to write

$$(\mathbf{I} + \mathbf{T}^{-1}\mathbf{V})^{-1} = \begin{pmatrix} \mathbf{P}_1 & \mathbf{P}_2 \\ \mathbf{P}_3 & \mathbf{P}_4 \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{Q}_3 & \mathbf{Q}_4 \end{pmatrix}, \quad (\text{A2})$$

where

$$\begin{aligned} (\mathbf{P}_1)_{n,m} &= \delta_{n,m} - \frac{(u - xv)}{x - x^{-1}} x^{-n} \delta_{0,m}, \\ (\mathbf{P}_2)_{n,m} &= -\frac{(xu - v)}{x - x^{-1}} x^{-n} \delta_{1,m}, \\ (\mathbf{P}_3)_{n,m} &= -\frac{(xu - v)}{x - x^{-1}} x^n \delta_{0,m}, \\ (\mathbf{P}_4)_{n,m} &= \delta_{n,m} - \frac{(u - xv)}{x - x^{-1}} x^n \delta_{1,m}. \end{aligned} \quad (\text{A3})$$

Since both \mathbf{P}_1^{-1} and \mathbf{P}_4^{-1} exist and can be obtained without too much difficulty, we write

$$\begin{aligned} \mathbf{Q}_1 &= (\mathbf{P}_1 - \mathbf{P}_2\mathbf{P}_4^{-1}\mathbf{P}_3)^{-1}, \\ \mathbf{Q}_2 &= \mathbf{P}_1^{-1}\mathbf{P}_2(\mathbf{P}_3\mathbf{P}_1^{-1}\mathbf{P}_2 - \mathbf{P}_4)^{-1}, \\ \mathbf{Q}_3 &= \mathbf{P}_4^{-1}\mathbf{P}_3(\mathbf{P}_2\mathbf{P}_4^{-1}\mathbf{P}_3 - \mathbf{P}_1)^{-1}, \\ \mathbf{Q}_4 &= (\mathbf{P}_4 - \mathbf{P}_3\mathbf{P}_1^{-1}\mathbf{P}_2)^{-1}. \end{aligned} \quad (\text{A4})$$

After some tedious but straightforward algebra, all the matrix elements of the above matrices can be calculated analytically. Together with (A1), we finally obtain (18) and (19).

APPENDIX B

The integrals involved in calculating (30) and (31) consist of two types: those along the real axis of x between $(-1, 1)$ and those along the unit semicircle above the real axis centered at the origin. The first type can be easily obtained using the standard residue theory. We here only show a typical integration of the second type. To obtain (31) we need to evaluate the following integral, after putting $x = e^{i\theta}$,

$$\text{Im} \int_0^\pi d\theta \sin \theta \frac{e^{in\theta}}{(e^{i\theta} - x_1)(e^{i\theta} - x_2)} e^{-E(\theta)t}. \quad (\text{B1})$$

Since both $|x_1|$ and $|x_2|$ are less than unity, we can use the expansion

$$\begin{aligned} & \text{Im} \frac{\sin \theta e^{in\theta}}{(e^{i\theta} - x_1)(e^{i\theta} - x_2)} \\ &= \text{Im} \frac{\sin \theta e^{i\theta(n-1)}}{x_1 - x_2} \left[\frac{1}{1 - x_1 e^{-i\theta}} - \frac{1}{1 - x_2 e^{-i\theta}} \right] \\ &= \text{Im} \sum_{k=1}^{\infty} \frac{x_1^k - x_2^k}{x_1 - x_2} e^{i\theta(n-1-k)} \sin \theta \\ &= \frac{1}{2} \sum_{k=1}^{\infty} \frac{x_1^k - x_2^k}{x_1 - x_2} [\cos(n-k-2)\theta \\ &\quad - \cos(n-k)\theta]. \end{aligned} \quad (\text{B2})$$

Substituting (B2) into (B1) and using the integral representation of the modified Bessel function

$$I_n(\tau) = \frac{1}{\pi} \int_0^\pi e^{\tau \cos \theta} \cos n\theta d\theta,$$

we obtain the last term in (31). Other integrals can be worked out in a similar fashion.

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