# Response functions of the diffusion model of one-dimensional disordered systems

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The configurational average response of discrete one-dimensional disordered systems modeled by the classical diffusion equation is investigated. Perturbation expansions of the system response functions based on the average deviation $\langle \Delta W \rangle$ of the nearest-neighbor interaction constants $W_n$ are developed in the frequency domain. It is shown that for probability distributions $\rho(W)$ such that $\langle W^{-1} \rangle$ is finite, a frequently applied effective-medium approximation is exact to second order in $\Delta W$ for all frequencies. The frequency dependence of the hopping conductivity is a second-order effect.

## I. INTRODUCTION

The response and transport properties of discrete one-dimensional systems are of interest in diverse fields of research. A simple mathematical model manifesting the observed response phenomena associated with many such systems is the classical equation

$$\frac{dX_n}{dt} = W_n(X_{n+1} - X_n) + W_{n-1}(X_{n-1} - X_n) \quad . \tag{1.1}$$

The nearest-neighbor interaction constants $W_n$, having units of reciprocal time, and the functions $X_n(t)$ are subject to numerous interpretations, depending on the physical system considered. Applications of (1.1) are well documented in the literature,[1,2] and need not be detailed here.

It is the purpose of this report to develop and compare perturbation and self-consistent effective-medium approximations (EMA) for the response functions of (1.1), and to calculate the hopping conductivity.

## II. PERTURBATION EQUATIONS

The Laplace transform of (1.1) with respect to the parameter $s$ is the matrix equation $H(s)\bar{X}(s) = X(0)$, where $\bar{X}(s)$ is a vector having components $\bar{X}_n(s)$ which are the transforms of $X_n(t)$, and $X(0)$ is a vector with components $X_n(0)$. The matrix $H(s)$ is a symmetric tridiagonal matrix with elements

$$H_{n,n} = W_n + W_{n-1} + s, \quad H_{n+1,n} = H_{n,n+1} = -W_n \quad , \tag{2.1}$$

and $H_{n,k} = 0$ otherwise. The response functions of the system are the matrix elements $G_{n,k} = (H^{-1})_{n,k}$.

For homogeneous systems with $W_n = W^0$, the response matrix $G^0 = [H^0(W^0)]^{-1}$ may be obtained by the projection-recurrence method.[3] The response functions $G^0_{n,k}$ for systems of infinite extent are

$$G^0_{n,k} = G^0_{k,n} = (2W^0 \sinh\theta)^{-1} e^{-(k-n)\theta} \quad \text{for } k \geq n \quad , \tag{2.2}$$

with

$$\cosh\theta = 1 + s(2W^0)^{-1} \quad . \tag{2.3}$$

To treat disordered systems, we define $\Delta W_n = W^0 - W_n$ and develop $G = H^{-1}$ in a Neumann series in $\Delta H(\Delta W)$,

$$G = G^0 + G^0 \Delta H G = G^0 + G^0 \sum_{k=0}^{\infty} (\Delta H G^0)^k \Delta H G^0 \quad . \tag{2.4}$$

Key steps in the evaluation of (2.4) to order $(\Delta H)^2$ are given in the Appendix. The average response $\langle G \rangle$, defined with respect to probability distributions $\rho(W)$, has matrix elements

$$\begin{aligned} \langle G_{n,k}(s) \rangle = G^0_{n,k} (1 &+ (\cosh\theta + 1)^{-1} [1 - (k-n)\sinh\theta] \epsilon \\ &+ \tfrac{1}{2} (\cosh\theta + 1)^{-2} \{3 - (k-n)\sinh\theta [\cosh\theta + 4 - (k-n)\sinh\theta]\} \epsilon^2 \\ &+ (\cosh\theta + 1)^{-2} (1 + \cosh\theta - \sinh\theta) [1 - (k-n)\sinh\theta] \delta^2) \quad \text{for } k \geq n \quad , \end{aligned} \tag{2.5}$$

with

$$\epsilon = \langle \Delta W \rangle / W^0, \quad \delta = [\langle (\Delta W)^2 \rangle - \langle \Delta W \rangle^2]^{1/2} / W^0 \quad . \tag{2.6}$$

The inverse transform of $\langle G_{n,k} \rangle$ in the low-frequency limit $s = i\omega \to 0$ manifests the $t^{-1/2}$ diffusive long-time behavior of $G^0_{n,k}(t)$. The general expression for $\langle G_{n,k}(t) \rangle$ is not evaluated, since the main emphasis here is to determine the frequency-dependent hopping conductivity, and to compare the perturbation results with the EMA response developed in Sec. III. It is emphasized that (2.5) is exact to second order in $\Delta W/W^0$; thus it should be quite accurate in modeling systems with a narrow distribution of interaction constants. Several physical systems to which (2.5) may be applied are discussed in Ref. 2. For example, the functions $\langle G_{n,k}\rangle$ are average transfer impedances of infinite ladder filters modeling inhomogeneous transmission lines and wave guides.[4]

The hopping conductivity $\sigma(s)$ is proportional to the mobility $\mu(s)$ given by[2]

$$\mu(s)=s^2\sum_{k=1}^{\infty}k^2\langle G_{0,k}(s)\rangle \quad . \tag{2.7}$$

Analysis of (2.7) using (2.5) yields the expression

$$\mu(s)=W^0[1-\epsilon-\delta^2+\delta^2F(s)], \tag{2.8}$$

$$\text{with } F(s)=[s/(s+4W^0)]^{1/2} \quad .$$

The real and imaginary parts of $F(s=i\omega)$, plotted in the Fig. 1, exhibit general characteristics of $\sigma(\omega)\sim\mu(\omega)$ for several low-dimensional conductors.[5,6] $\mathrm{Re}\sigma$ increases monotonically from a nonzero dc value to a constant in the high-frequency limit $\omega'=\omega/4W^0>>1$, and $\mathrm{Im}\sigma>0$ approaches zero in both low- and high-frequency limits, with a maximum at $\omega=2.2W^0$. Much of this general behavior is also present in the random-bond percolation model in one dimension[7] and in three dimensions.[7,8]

The low-frequency dependence $\mathrm{Re}\sigma(\omega)-\sigma(0)\sim\omega^\beta$ differs for different classes of probability density models. For $\rho(W)$ such that $\langle W^{-1}\rangle$ is finite, (2.8) yields $\sigma(0)>0$ and $\beta=0.5$. In the percolation model, $\sigma(0)=0$ and $\beta=2$.[7] In thermally activated hopping models with $\rho(W)\sim W^{-\alpha}$, one finds that $\sigma(0)=0$ and $\beta=\alpha/(2-\alpha)$ when $0<\alpha<1$.[2,9] Measurements of $\sigma(\omega)$ yield different values of $\sigma(0)$ and $\beta$, depending on a number of physical parameters. For example, $NbSe_3$ exhibits $\sigma(0)>0$ and $\beta=1$ at temperature $T=42$ K, as explained by a charge-density-wave model.[5] In hollandite, measurement of $\sigma(\omega)$ from $T=150$ to 280 K gives a range $0.2<\beta<0.5$, with the larger value of $\beta$ corresponding to the smaller temperature.[9] The conductivity of doped silicon shows an $\omega^\beta$ dependence, with $\beta$ a function of doping density. For a doping density of $2.7\times10^{17}$ $cm^{-3}$ boron or phosphorus, the value of $\beta=0.5$.[8]

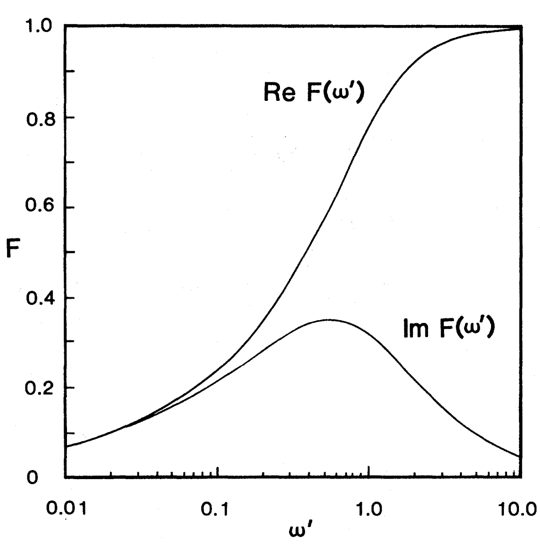


FIG. 1. The real and imaginary parts of the ac conductivity are plotted as a function of the normalized frequency $\omega'=\omega/4W^0$.

## III. EFFECTIVE-MEDIUM APPROXIMATION

The EMA considered here is based on an idea introduced by Soven as the coherent potential approximation to obtain a tractable theory for calculating the electronic spectra of random metallic alloys.[10] This self-consistent approximation theory has been widely applied to disordered systems, with considerable success in qualitatively predicting characteristic phenomena.[6,8–11]

Briefly, the formulation begins by casting (2.4) in the form

$$G=G^x+G^xG^xTG^x, \text{ with } T=(I-\Delta HG^x)^{-1}\Delta H \quad . \tag{3.1}$$

The matrix $G^x$, defined by $G^x=[H^x(W^x)]^{-1}$, is an effective-medium response matrix which is a function of a homogeneous effective-medium interaction constant $W^x=W_n+\Delta W_n$. The function $W^x$ is determined self-consistently from the condition $\langle T\rangle=0$, i.e., $\langle G\rangle=G^x$.

The matrix $T$ is easily evaluated whenever $\Delta H=\Delta cQ$, with $\Delta c$ a scalar, and rank $Q=1$, i.e., $Q$ has the form $Q=|q\rangle\langle r|$. In this case, $\Delta HG^x$ is an eigenoperator of $\Delta H$ and $T$ is given by

$$T=\Delta c(1-\Delta c\langle r|G^x|q\rangle)^{-1}Q \quad . \tag{3.2}$$

Equation (3.2) is valid for a single parameter change in numerous physical systems. It holds for all passive interaction constants in any discrete linear system, and for many active components such as controlled sources in analog electrical networks.

In the problem considered here, a change $\Delta W_n$ in a random bond connecting nodes $n$ and $n+1$ is manifested by the change $\Delta H=\Delta W_nQ_n$. The matrix $Q_n$ is a symmetric rank one matrix given by $Q_n=|q\rangle\langle q|$, with $q\rangle=|n\rangle-|n+1\rangle$. Using (2.2) in (3.2) with $\theta$ replaced by $\theta(W^x)$ to evaluate $\langle q|G^x|q\rangle$, the effective-medium condition $\langle T\rangle=0$ assumes the form

$$\int_0^\infty \frac{dW\rho(W)(W^x-W)}{s[1+(1+4W^x/s)^{1/2}]+4W}=0 \ . \qquad (3.3)$$

Equation (3.3) defines $W^x$ with respect to a probability distribution density $\rho(W)$. The EMA response functions of the system are given by

$$G^x_{n,k}(s)=\exp[-(k-n)\cosh^{-1}(1+s/2W^x)] \times [s(s+4W^x)]^{-1/2} \ . \qquad (3.4)$$

To test the accuracy of the EMA, we compare $G^x_{n,k}$ with the perturbation expression (2.5) for $\langle G_{n,k}\rangle$. For probability densities $\rho(W)$ such that $\langle W^{-1}\rangle$ is finite, the integrand in (3.3) is expanded in a power series in $\Delta W/W^0=(W^0-W)/W^0$. The resulting expression for $W^x$ to second order is

$$W^x/W^0=1-\epsilon-\{1-[s(s+4W^0)^{-1}]^{1/2}\}\delta^2 \ , \qquad (3.5)$$

with $\epsilon$ and $\delta$ defined in (2.6). Substitution of $W^x$ into (3.4) and comparing $G^x_{n,k}$ with $\langle G_{n,k}\rangle$ in (2.5) shows exact agreement in all terms for all values of $s$. As a verification of consistency, note that the expression for $W^x(s)$ is identical to the perturbation result (2.8) for $\mu(s)$. Although some agreement is expected, since the first correction to the EMA is of fourth order in the single-bond matrices $T_n$,[5] this appears to be the first application of an EMA shown explicitly to be exact to second order in a perturbation parameter.

The conductivity of the quasi-one-dimensional conductor quinolinium dietetracyanoquinodimethanide [Qn(TCNQ)$_2$] has recently been accurately modeled within the EMA using a thermally activated hopping distribution $\rho(W)\sim W^{-\alpha}$.[6] The range of $W$ is restricted to $W_{\min}<W<W_{\max}$, with $W_{\min}$ and $W_{\max}$ temperature dependent. Since the relative width $(W_{\max}-W_{\min})/W_{\max}$ decreases with increasing temperature,[6] the conductivity $\sigma(s)\sim\mu(s)=W^x(s)$ given by (2.8) or (3.5) is the asymptotically exact expression for $\sigma(s)$ for all $s=i\omega$ in the high-temperature limit.

## IV. CONCLUSION

The perturbation theory response of the discrete classical diffusion equation serves as a benchmark for approximate theories using this model to explain the ac response of low-dimensional conductors. It was shown that the widely applied effective-medium approximation is extremely good for narrow interaction constant distributions of density $\rho(W)$ with $\langle W^{-1}\rangle$ finite. Exact agreement with second-order perturbation theory was shown for all such distributions for arbitrary values of the Laplace parameter $s$. In contrast to the complicated dependence of the response functions on $s$, the conductivity has a relatively simple dependence on $s$, which appears only in a term proportional to the variance in the interaction constants. Thus, for systems for which a narrow distribution model is applicable, a careful measurement of $\sigma(\omega)-\sigma(0)$ is needed to observe the ac part of the conductivity.

## APPENDIX

Assuming that $W_n$ is an independently distributed random variable, the configurational average matrix elements in Eq. (2.4), calculated to order $(\Delta H)^2$ are

$$\begin{aligned}\langle G_{n,m}(s)\rangle = {} & G^0_{n,m}+\langle\Delta W\rangle\sum_k G^0_{n,k}(-G^0_{k-1,m}+2G^0_{k,m}-G^0_{k+1,m})\\ & +\langle\Delta W\rangle^2\sum_k\sum_{k'}G^0_{n,k}(-G^0_{k-1,k'}+2G^0_{k,k'}-G^0_{k+1,k'})(-G^0_{k'-1,m}+2G^0_{k',m}-G^0_{k'+1,m})\\ & +[\langle(\Delta W)^2\rangle-\langle\Delta W\rangle^2]\sum_k G^0_{n,k}[(G^0_{k,k}-2G^0_{k-1,k}+G^0_{k-1,k-1})(G^0_{k,m}-G^0_{k-1,m})\\ & +(G^0_{k,k}-2G^0_{k,k+1}+G^0_{k+1,k+1})(G^0_{k,m}-G^0_{k+1,m})] \ . \end{aligned} \qquad (A1)$$

Using the identity

$$-G^0_{k-1,n}+2\cosh\theta G^0_{k,n}-G^0_{k+1,n}=\delta_{n,k}/W^0 \ ,$$

which follows from $H^0G^0=I$, leads to

$$\begin{aligned}\langle G_{n,m}(s)\rangle = {} & G^0_{n,m}+[G^0_{n,m}+2W^0(1-\cosh\theta)R_1(n,m)]\epsilon\\ & +\{G^0_{n,m}+4W^0(1-\cosh\theta)R_1(n,m)+[2W^0(1-\cosh\theta)^2R_2(n,m)]\}\epsilon^2\\ & +(1-e^{-\theta})(\sinh\theta)^{-1}[G^0_{n,m}+2W^0(1-\cosh\theta)R_1(n,m)]\delta^2 \ , \end{aligned} \qquad (A2)$$

where

$$\epsilon=\langle\Delta W\rangle/W^0,\quad \delta=[\langle(\Delta W)^2\rangle-\langle\Delta W\rangle^2]^{1/2}/W^0\ ,\quad R_1(n,m)=\sum_{k=1}^{\infty}G_{n,k}^0G_{k,m}^0\ ,\quad R_2(n,m)=\sum_{k=1}^{\infty}\sum_{k'=1}^{\infty}G_{n,k}^0G_{k,k'}^0G_{k',m}^0\ . \tag{A3}$$

The sums $R_1$ and $R_2$ are arithmetico-geometric progressions in $e^{\pm\theta}$. Evaluation is tedious because the exponent in $G_{k,k'}^0\sim e^{\pm(k-k')\theta}$ changes sign at $k=k'$. Analysis gives

$$2W^0\sinh\theta R_1(n,m)=G_{n,m}^0(\cosh\theta/\sinh\theta+m-n)\ , \tag{A4}$$

and

$$(2W^0\sinh\theta)^2R_2(n,m)=G_{n,m}^0[(\cosh\theta/\sinh\theta)^2+\tfrac{1}{2}(\sinh\theta)^{-2}+\tfrac{1}{2}(m-n)(3\cosh\theta/\sinh\theta+m-n)]\ .$$

Substituting (A4) into (A2) gives (2.5).

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