Role of pinning potentials in heat transport through disordered harmonic chains

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The role of quadratic on-site pinning potentials on determining the size (N) dependence of the disorder averaged steady state heat current $\langle J \rangle$ in an isotopically disordered harmonic chain connected to stochastic heat baths is investigated. For two models of heat baths, namely white noise baths and Rubin's model of baths, we find that the N dependence of $\langle J \rangle$ is the same and depends on the number of pinning centers present in the chain. In the absence of pinning, $\langle J \rangle_{Fr} \sim 1/N^{1/2}$ while in the presence of one or two pins $\langle J \rangle_{Fi} \sim 1/N^{3/2}$. For a finite ($n$) number of pinning centers with $2 \leqslant n \ll N$ we provide heuristic arguments and numerical evidence to show that $\langle J \rangle_n \sim 1/N^{n-1/2}$. We discuss the relevance of our results in the context of recent experiments.

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Since the seminal paper of Anderson [1], the physics of localization in disordered systems has now been studied for over half a century [2–5]. Recently there has been a renewed interest in this field with a lot of work on some open questions such as, for example, the effect of interactions on localization [6–8], and the metal-insulator transition in two dimensions [9]. A number of recent experiments have also reported detailed studies on localization in varied systems such as heat conduction in a isotopically disordered nanotube [10], electrons in a disordered carbon nanotube [11], photons in a waveguide [12], and sound localization in elastic networks [13]. The field is thus still filled with interesting questions and puzzles. Here in this paper we point out that even the simple problem of heat conduction in a one-dimensional disordered harmonic lattice has surprises.

It is well known that all the eigenstates of an electron in a one-dimensional disordered potential are localized. The electrical current thus decays exponentially with wire length, making it an insulator. In contrast, in phononic systems, for example, a disordered harmonic chain, long wavelength modes are extended and can conduct a significant amount of heat. How good a heat conductor then is the disordered harmonic chain? The obvious question to ask is the system size (N) dependence of the disorder averaged steady state heat current which we will denote by $\langle J \rangle$. It is expected that this has the form $\langle J \rangle \sim 1/N^{1-\alpha}$ so that the conductivity scales as $\kappa \sim N^{\alpha}$. The dependence of α on the choice of heat baths and boundary conditions has been somewhat puzzling and has caused some amount of confusion. We note that heat conduction in this system is nondiffusive and correspondingly $\alpha \neq 0$.

We briefly review earlier work on this problem [14]. In an important work on the localization of normal modes in the isotopically disordered harmonic chain (IDHC), Matsuda and Ishii [3] (MI) showed that normal modes with frequencies $\omega \lesssim \omega_d$ were extended. For a harmonic chain of length N, given the average mass $m = \langle m_l \rangle$, the variance $\sigma^2 = \langle (m_l - m)^2 \rangle$, and interparticle spring constant k, it was shown that

$$\omega_d \sim \left(\frac{km}{N\sigma^2} \right)^{1/2}. \tag{1}$$

They also evaluated expressions for thermal conductivity of a finite disordered chain connected to (a) white noise baths and (b) baths modeled by semi-infinite ordered harmonic chains (Rubin's model of baths). In the following we will also consider these two models of baths and refer to them as model (a) and model (b). For model (a) MI used fixed boundary conditions (BCs) and the limit of weak coupling to baths, while for case (b) they considered free BCs and this was treated using the Kubo formalism. They found $\alpha = 1/2$ in both cases, a conclusion which we will show is incorrect. The other two important theoretical papers on heat conduction in the disordered chain are those by Rubin and Greer (RG) [15] who considered model (b) and of Casher and Lebowitz (CL) [16] who used model (a) for baths. RG obtained a lower bound $\langle J \rangle \geqslant 1/N^{1/2}$ and gave numerical evidence for an exponent $\alpha = 1/2$ and this was later proved rigorously by Verheggen [17]. On the other hand, for model (a), CL found a rigorous bound $\langle J \rangle \geqslant 1/N^{3/2}$ and simulations by Visscher with the same baths supported the corresponding exponent $\alpha = -1/2$. In a more recent work [18], one of us (A.D.) gave a unified treatment of the problem of heat conduction in disordered harmonic chains connected to baths modeled by generalized Langevin equations and showed that models (a) and (b) were two special cases. An efficient numerical scheme was proposed and used to obtain the exponent α and it was established that $\alpha = -1/2$ for model (a) (with fixed BC) and $\alpha = 1/2$ for model (b) (with free BC). It was also pointed out that, in general, α depended on the spectral properties of the baths.

Here we apply the same formulation as developed in [18] to understand in detail the role of BCs (and more generally the presence of pinning potentials) on heat transport in the IDHC connected to either white noise [model (a)] or Rubin baths [model (b)]. We show that with the same kind of pinning, the exponent α is the same for the two different bath models. The pinning potentials strongly scatter low frequency waves and hence can be expected to lower the heat current. Surprisingly, we find that even the exponent α changes with the number of pinning centers. We also provide expressions for the asymptotic value of $\langle J \rangle$ for various cases.

The Hamiltonian of the IDHC considered here is

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N-1} \frac{1}{2} k (x_{l+1} - x_l)^2 + \frac{1}{2} k' (x_1^2 + x_N^2), \tag{2}$$

where $\{x_l, p_l\}$ denote the displacement and momentum of the particle at lattice site l. The random masses $\{m_l\}$ are chosen

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from a uniform distribution between $(m-\Delta)$ to $(m+\Delta)$. The strength of on-site potentials at the boundaries is k'. The particles at two ends are connected to heat baths at temperature T_L and T_R. The heat reservoirs are modeled by generalized Langevin equations [18–20]. The steady state classical heat current through the chain is given by

$$J = \frac{k_B(T_L - T_R)}{4\pi} \int_{-\infty}^{\infty} d\omega \mathcal{T}_N(\omega), \tag{3}$$

where

$$\mathcal{T}_N(\omega) = 4\Gamma^2(\omega)|G_{1N}(\omega)|^2, \quad \hat{G}(\omega) = \hat{Z}^{-1}/k,$$

and

$$\hat{Z} = [-\omega^2\hat{M} + \hat{\Phi} - \hat{\Sigma}(\omega)]/k,$$

where $\hat{M}$ and $\hat{\Phi}$ are, respectively, the mass and force matrix for the harmonic chain and $\hat{G}$ is the Green's function of the chain connected to baths. The self-energy correction in the Green's function $\hat{\Sigma}$, coming from the baths, is an $N\times N$ matrix whose only nonzero elements are $\Sigma_{11}=\Sigma_{NN}=\Sigma(\omega)$ and $\Gamma(\omega)=\mathrm{Im}[\Sigma]$. For white noise baths $\Sigma(\omega)=-i\gamma\omega$ where γ is the coupling strength with the baths, while in the case of Rubin's baths

$$\Sigma(\omega) = k\{1 - m\omega^2/2k - i\omega(m/k)^{1/2}[1 - m\omega^2/(4k)]^{1/2}\}.$$

We have assumed that the RG bath has spring constant k and equal masses m. We note that $\mathcal{T}_N(\omega)$ is the transmission coefficient of phonons through the disordered chain. To extract the asymptotic N dependence of $\langle J\rangle$ we need to determine the Green's function element $G_{1N}(\omega)$. It is convenient to write the matrix elements $Z_{11}=-m_1\omega^2/k+1+k'/k-\Sigma/k=-m_1\omega^2/k+2-\Sigma'$ where $\Sigma'=\Sigma/k-k'/k+1$ and similarly $Z_{NN}=-m_N\omega^2/k+2-\Sigma'$. Following the techniques used in [16,18] we have

$$|G_{1N}(\omega)|^2 = k^{-2}|\Delta_N(\omega)|^{-2} \tag{4}$$

with

$$\Delta_N(\omega) = D_{1,N} - \Sigma'(D_{2,N} + D_{1,N-1}) + \Sigma'^2 D_{2,N-1},$$

where $\Delta_N(\omega)$ is the determinant of $\hat{Z}$ and the matrix elements $D_{l,m}$ are given by the following product of (2×2) random matrices $\hat{T}_l$:

$$\hat{D} = \begin{pmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{pmatrix} = \hat{T}_1\hat{T}_2\cdots\hat{T}_N, \tag{5}$$

where

$$\hat{T}_l = \begin{pmatrix} 2 - m_l\omega^2/k & -1 \\ 1 & 0 \end{pmatrix}.$$

We note that the information about bath properties and boundary conditions are now contained entirely in $\Sigma'(\omega)$ while $\hat{D}$ contains the system properties. It is known that $|D_{l,m}|\sim e^{cN\omega^2}$ for $|l-m|\sim N$ [3], where c is a constant, and so we need to look only at the low frequency $(\omega \lesssim 1/N^{1/2})$ form of Σ'. We now proceed to examine various cases. For model

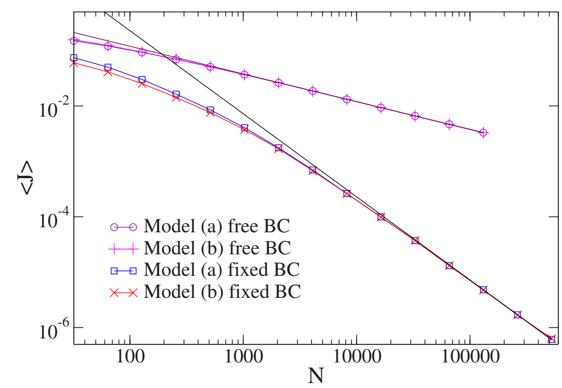

FIG. 1. (Color online) Plot of $\langle J\rangle$ vs N for free BCs $(n=0)$ and fixed BCs $(n=2)$. Results are given for both models (a) and (b) of baths. The two straight lines correspond to the asymptotic expressions given in Eqs. (10) and (11). We used parameters $m=1$, $\Delta=0.5$, $k=1$, $\gamma=1$, $T_L=2$, $T_R=1$, and $k_o=1$. The error in the measurements is much smaller than the size of the symbols.

(a) free BCs correspond to $k'=0$ and so $\Sigma'=1-i\gamma\omega/k$ while for model (b) free boundaries correspond to $k'=k$ and this gives, at low frequencies, $\Sigma'=1-i(m/k)^{1/2}\omega$. Other values of k' correspond to pinned boundary sites with an on-site potential $k_o x^2/2$ where $k_o=k'$ for model (a) and $k_o=k'-k$ for model (b). The main difference, from the unpinned case, is that now $\mathrm{Re}[\Sigma']\neq 1$. The arguments of [18] then immediately give $\alpha=1/2$ for free BCs and $\alpha=-1/2$ for fixed BCs for both bath models. The arguments consisted of two parts: (i) it was observed numerically that the transmission coefficients at low frequencies for the ordered and disordered chain were almost the same, and (ii) an asymptotic analysis was then carried out for the ordered case, for which $\mathcal{T}$ could be obtained exactly for any bath spectral properties (an improved version of those arguments is given below).

For the choice of parameters $\gamma=(mk)^{1/2}$, the imaginary part of Σ' is the same for both bath models, and we expect, for large system sizes, the actual values of the current to be the same in both cases. This can be seen in Fig. 1 where we show the system size dependence of the current for the various cases. The current was evaluated numerically using Eq. (3) and averaging over many realizations ($\sim 4-100$). We also show the exact asymptotic forms for the current which we will discuss later. Note that for free BCs, the exponent $\alpha=1/2$ settles to its asymptotic value at relatively small values $(N\sim 10^3)$ while, with pinning, we need to examine much longer chains $(N\sim 10^5)$. We also find that the presence of a single pinning center in the IDHC is sufficient to change the value of α from $1/2$ to $-1/2$ (see Fig. 2). These results clearly show that, for both models (a) and (b), the exponent α is the same and is controlled by the presence or absence of pinning in the IDHC.

Next we try to better understand the above results. As mentioned before only modes $\omega \lesssim \omega_d$ are involved in conduction. It was noted in [18] that in this low frequency regime we can approximate $\langle \mathcal{T}_N(\omega)\rangle$ by the transmission coefficient of the ordered chain $\mathcal{T}_N^O(\omega)$. We then obtain

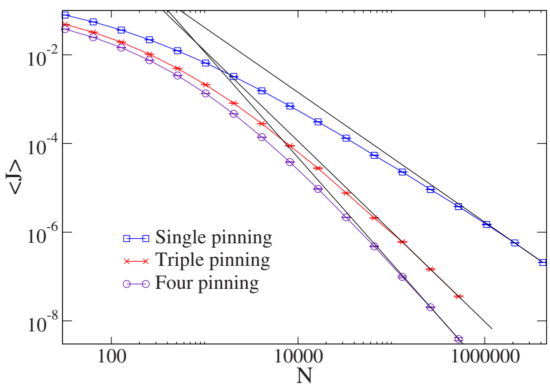

FIG. 2. (Color online) Plot of $\langle J\rangle$ vs N for $n=1,3,4$ pinning centers for model (b). Parameters are same as in Fig. 1 and for these parameters model (a) results are almost indistinguishable for $N>10^3$. The straight lines have slopes -1.47, -2.03, and -2.38. The error bars shown are for disorder average and are of the same order as numerical errors.

$$\langle J\rangle \sim (T_L-T_R)\int_0^{\omega_d}\mathcal{T}_N^O(\omega)d\omega. \tag{6}$$

For model (a), $\mathcal{T}_N^O$ in the limit $N\to\infty$ is effectively given by [21]

$$\mathcal{T}^O(\omega)=\frac{\gamma\omega^2\sqrt{4mk-m^2\omega^2}}{k'^2+[\gamma^2+m(k-k')]\omega^2}. \tag{7}$$

We then find for free BCs ($k'=0$), $\mathcal{T}^O(\omega)\sim 1$ while for fixed BCs ($k'\neq 0$), $\mathcal{T}^O(\omega)\sim\omega^2$. Using Eq. (6) then immediately gives the asymptotic N dependence for the two BCs. Our results are valid even in the weak coupling limit $\gamma\ll 1$ and this means that the result given by MI for model (a) in the weak coupling limit is incorrect. Our numerics supports this conclusion. We also compute the transmission coefficient of the ordered chain (as $N\to\infty$) in the presence of a single pinning at one boundary,

$$\mathcal{T}_\infty^O(\omega)=\frac{2\gamma\omega^2\sqrt{4mk-m^2\omega^2}}{\sqrt{4\omega^4\Lambda^2+k'\Omega(k'\Omega+4\omega^2\Lambda)}},$$

with

$$\Lambda=\gamma^2+km,\quad \Omega=k'-m\omega^2, \tag{8}$$

and we again find $\mathcal{T}^O\sim\omega^2$, for $k'\neq 0$. This confirms our numerics that the asymptotic N dependence of $\langle J\rangle$ is analogous for the IDHC with single or double pinning centers. For model (b), the transmission coefficient of the ordered chain, pinned at the two boundary sites with $k_o=k'-k$, is given effectively by (as $N\to\infty$)

$$\mathcal{T}^O(\omega)=\frac{2k^2\sin^2 q}{2k^2\sin^2 q+k_o^2}, \tag{9}$$

where $\omega=2(k/m)^{1/2}\sin(q/2)$. As expected, for $k_o=0$ we have $\mathcal{T}^O=1$ while for $k_o\neq 0$, $\mathcal{T}^O\sim\omega^2$. The above qualitative analysis thus shows that the effect of introducing pinning potentials is to pinch the band of conducting modes (between $0-\omega_d$) from the zero frequency side and thus lower $\langle J\rangle$.

Our asymptotic analysis also allows us to make predictions, on the dependence of $\langle J\rangle$, on various system parameters such as mass variance, spring constant, etc. Here we denote $\langle J\rangle_{Fr}$ for $\langle J\rangle$ in the absence of pinning while $\langle J\rangle_{Fi}$ represents $\langle J\rangle$ in the presence of double pinnings at the boundaries. From Eq. (6) and the forms of $\mathcal{T}^O(\omega)$ in various cases we get

$$\langle J\rangle_{Fr}=Ac\frac{k_B(T_L-T_R)}{\pi}\left(\frac{km}{N\sigma^2}\right)^{1/2}, \tag{10}$$

$$\langle J\rangle_{Fi}=A'c'\frac{k_B(T_L-T_R)}{\pi}\left(\frac{km}{N\sigma^2}\right)^{3/2}, \tag{11}$$

where $c=2\gamma(mk)^{1/2}/(\gamma^2+mk)$, 1 for model (a) and model (b), respectively. For fixed boundaries we have $c'=\gamma(mk)^{1/2}/k_o^2$, mk/k_o^2 for model (a) and model (b), respectively. A,A' are constant numbers. We find that for model (b) our numerical results agree with an exact expression for $\langle J\rangle_{Fr}$ due to Papanicolau (apart from a factor of 2π) and this gives $A=\pi^{3/2}\int_0^\infty dt[t\sinh(\pi t)]/[(t^2+1/4)^{1/2}\cosh^2(\pi t)]\approx 1.084\,17$ (see [17]). We note that this differs from the expression given in [3]. For fixed boundaries we find numerically that $A'\approx 17.28$ and the fit is shown in Fig. 1. Based on our analytical and numerical results, we believe that the expression in [17] is in error by a 2π factor.

Until now, using numerical results and heuristic arguments, we have arrived at the result that for a IDHC, in the absence of any pinning potential, $\alpha=1/2$ while the presence of one or two pinned sites changes the exponent to $\alpha=-1/2$. This is true both for white noise and Rubin's bath. It is natural to now asks what happens in the presence of more numbers of pinning centers. It is expected that more pinning centers will lead to enhanced scattering of low frequency phonons and decrease the heat current but it is not obvious as to whether the exponent α changes. For a finite fraction of sites on the lattice having pinning potentials, it is known that $\langle J\rangle\sim e^{-cN}$ [8]. Here we investigate the case with a finite number, say n, of pinning sites. Numerically it becomes difficult to determine α for $n>4$ as, with more pins, the heat current becomes very small at large system sizes and numerical errors become significant. In Fig. 2 we show numerical results for $n=3,4$, where the extra pinning potentials with $k_o=1$ are placed in the bulk of the chain with equal separations. We find $\alpha\approx -1.03,-1.38$, respectively for $n=3,4$, which are clearly different from the $n=1,2$ value $\alpha=-0.5$. Let us now see what our earlier heuristic arguments give, for $n=3$. We again find that the low frequency behaviors of $\Delta_N(\omega)$ are similar for the disordered and ordered lattices. Let us therefore find the form of Δ_N for the ordered case. Let $N=2M+1$ with the 1st, $(M+1)$th, and Nth sites being pinned. Except for $\hat{T}_{M+1}=\hat{T}'$ all the other $\hat{T}_l$s' are identical and given by $\hat{T}$, say. If we denote $\hat{D}_N=\hat{T}^N$ and $\hat{D}'_N=\hat{T}^M\hat{T}'\hat{T}^M=\hat{D}_M\hat{T}'\hat{D}_M$, then using the fact that for the ordered lattice $D_{1N}=\sin q(N+1)/\sin(q)$, where $\cos(q)=1-m\omega^2/(2k)$, and carrying out the matrix multiplications above we find that at low frequencies D'_{1N} is larger than D_{1N} by a factor $\sim 1/\sin(q)\sim 1/\omega$. This means that $\mathcal{T}_N$ for the three-pin case will have an extra factor of ω^2 compared to the two-pin case. Correspondingly one expects, using Eq. (6), an exponent $\alpha = -3/2$. The argument can be extended to the case of $n \geq 2$ pins (two of which are in the boundaries) in which case we get

$$\alpha = 3/2 - n. \tag{12}$$

Our numerical results for $n=3,4$ (see Fig. 2) are consistent with this prediction though we are not able to verify the precise value of the exponent.

Finally we note that the calculation by CL [16] for the lower bound on current, in the case of two pinning centers (fixed boundaries) in model (a), can be extended to the case with more pins. The argument by CL consists in evaluating $\langle D_{1N}^2 \rangle$ by looking at the disorder averaged direct product $\langle \hat{D} \otimes \hat{D} \rangle = \Pi_l \langle \hat{Q}_l \rangle$ where $\hat{Q}_l = \hat{T}_l \otimes \hat{T}_l$. In the CL case $\langle \hat{Q}_l \rangle = \hat{Q}$ for all $\hat{Q}$ and an analysis of the eigenvalues of $\hat{Q}$ led to the result $\langle D_{1N}^2 \rangle \sim e^{cN\omega^2}$. In our case, say for the case of $n=3$ with an additional pinning at site $l=M+1$, $\langle \hat{Q}_{M+1} \rangle = \hat{Q}'$ is different and we have $\langle \hat{D} \otimes \hat{D} \rangle = \hat{Q}^M \hat{Q}' \hat{Q}^M$. A careful analysis of this then gives $\langle D_{1N}^2 \rangle \simeq \omega^{-2} e^{cN\omega^2}$. Using this in Eq. (3) gives $\langle J \rangle_3 \geq C \int_0^\infty d\omega \omega^4 e^{-cN\omega^2} \sim O[N^{-5/2}]$, where c and C are constants. In general we get $\langle J \rangle_n \geq O[N^{-n+1/2}]$ for $2 \leq n \ll N$.

Quantum case. For a Hamiltonian of the form of Eq. (2) where now $\{x_l, p_l\}$ are Heisenberg operators, the steady state quantum heat current through the IDHC in the linear response regime is given by

$$J_q = \frac{k_B(T_L - T_R)}{4\pi} \int_{-\infty}^{\infty} d\omega \mathcal{T}_N(\omega) \left(\frac{\hbar\omega}{2k_B T} \right)^2 \operatorname{cosech}^2 \left(\frac{\hbar\omega}{2k_B T} \right),$$

where $\mathcal{T}_N(\omega)$ is the same as Eq. (3) and $T=(T_L+T_R)/2$. Following our derivation for the classical system we see that the asymptotic N dependence of $\langle J_q \rangle$ is determined by $\mathcal{T}_N(\omega)$ which is here exactly the same as the classical case. For any fixed temperature, however small, at sufficiently large system sizes we will have $\hbar\omega_d \ll k_B T$, and hence within this cutoff frequency the factor $(\hbar\omega/k_B T)^2 \operatorname{cosech}(\hbar\omega/k_B T)^2 \to 1$. Hence for large system sizes we always get the classical result. The approach to the asymptotic behavior though will be different.

Discussion. In real experiments heat baths usually have a finite bandwidth making the noise correlated, as in Rubin's model. Here we have shown that for heat conduction in the IDHC these noise correlations do not affect the exponent α [note that a bath for which $\Sigma(\omega)$ depends nonlinearly on ω at small frequencies can affect α]. We have elucidated the role of boundary conditions and shown that the actual value of α depends on the number of pinned sites. Our results are also valid for bond disorder. We have provided explicit expressions for the currents which, apart from giving the system size dependence, also give the dependence on various other parameters such as mass variance, coupling to baths, etc. We also emphasize that heat conduction through IDHC is nondiffusive. Our physical understanding is as follows. In the presence of mass or bond disorder phonons are scattered coherently giving rise to localization and low transmission. Long wavelength phonons with $\omega \lesssim \omega_d$ [see Eq. (1)] are relatively unaffected and dominate heat conduction in such disordered materials. Now the introduction of pinning centers causes strong scattering of even the low frequency modes and, as we have shown, significantly reduces the current. We obtain the surprising and nontrivial result that the exponent α giving the system size dependence of current changes linearly with the number of pinning centers. There are now experimental measurements of heat conduction in one-dimensional systems such as nanotubes and nanowires [10,22] and molecular wires [23]. At low temperatures one can neglect anharmonic effects and it will be interesting to see if our prediction of the strong reduction of heat current, by substrate potentials at localized points on a disordered wire, can be observed. While our results are for a simple classical model we expect the effect of pinning to be quite generic and should be true for systems with more complicated phonon dispersions. It will be interesting to see the effect of pinning potentials in heat conduction in two and three dimensions.

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