One dimension. Thermodynamics, kinetics, eigenstates, and universality

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Different physical problems in one dimension are related to the recurrence relation, whose solution at most linearly increases with the length of the system. In particular, limitations on the universality relation in localization are presented; phonon localization length, spectrum, and eigenstates are determined.

I. INTRODUCTION

Many one-dimensional (1D) problems in thermodynamics and kinetics reduce to the evaluation of the product of transfer matrices. The problems include a quantum particle in a given potential[1]; the Anderson model with diagonal and/or off-diagonal disorder; the Bloch electron in a magnetic field[2]; phonons in a harmonic chain[3]; classical diffusion; Ising alloys, ferromagnetics, antiferromagnetics, and ferrimagnetics[4]; DNA thermodynamics.[5] They are most interesting in random and quasiperiodic systems. But then they are most difficult, since the value of the product of matrices may exponentially increase with their number. In this case the possible localization of eigenstates may be of special interest. However, a straightforward calculation of eigenstates in, e.g., a harmonic chain of 1000 random force constants reduces to eigenstates of 1000×1000 matrix. In this paper I reduce the calculation of the product of arbitrary (complex) 2×2 matrices to the (real) recurrence relation directly for the exponent at most linearly increasing with the number of matrices. This maps all indicated problems on each other. To demonstrate how simple and efficient are the calculations, I show the limitations on the universality in 1D localization. The calculations are so accurate that they allow one to observe extraordinary narrow resonances of the wave transmission at eigenenergies. In this way, one may determine the eigenenergies. Then the recurrence relation determines the eigenfunctions and their localization. I demonstrate it on the phonon spectrum of a 1D random chain.

II. SCHRÖDINGER EQUATION; LOCALIZATION AND UNIVERSALITY

First consider the 1D Schrödinger equation with nonoverlapping potentials:

$$\psi''(x)+\left[k^2-\sum_\nu V_\nu(X-X_\nu)\right]\psi(x)=0 \ , \qquad (1)$$

where $x_{\nu+1}>x_\nu$. Between each x_ν and $x_{\nu+1}$ there is a region (maybe infinitesimally small), where the potential is zero. In this region

$$\psi=\alpha_\nu^+\exp(ikx)+\alpha_\nu^-\exp(-ikx) \ .$$

Suppose a single potential $V_\nu(x-x_\nu)$ leads to the transmission coefficient

$$\tau_\nu\equiv\cos(h_\nu)\exp(i\beta_\nu)$$

and the reflection coefficient

$$\rho_\nu\equiv\sin(h_\nu)\exp(i\beta_\nu-i\gamma_\nu) \ ,$$

where $|h_\nu|\leq\pi/2$. When $V_\nu(x-x_\nu)=\Upsilon_\nu\delta(x-x_\nu)$, then

$$\tan h_\nu=v_\nu/2k \ ; \ \ \beta_\nu=h_\nu-ka_\nu \ ; \qquad \gamma_\nu=\pi/2+ka_\nu \ ; \ \ a_\nu=x_\nu-x_{\nu-1} \ . \qquad (2)$$

In a general case, a simple calculation leads to

$$\alpha_L=\exp(-i\hat{k}x_L)\theta_L\theta_{L-1}\ldots\theta_1\alpha_0 \ ,$$

$$\alpha_\nu=\begin{pmatrix}\alpha_\nu^+\\ \alpha_\nu^-\end{pmatrix}, \ \ \hat{k}=\begin{pmatrix}k & 0\\ 0 & -k\end{pmatrix} \ , \qquad (3)$$

$$\theta_\nu=\begin{pmatrix}[\cos(h_\nu)]^{-1}\exp(-i\beta_\nu) & \tan(h_\nu)\exp(-i\gamma_\nu)\\ \tan(h_\nu)\exp(i\gamma_\nu) & [\cos(h_\nu)]^{-1}\exp(i\beta_\nu)\end{pmatrix} . \qquad (4)$$

Here h_ν determines the transmission: $|\tau_\nu|^2=\cos^2 h_\nu$, while β_ν and γ_ν determine the phase shifts for the waves reflected and transmitted by a single potential. Equation (4) is a general presentation of a transfer matrix. So one may investigate how the resistance of a random system depends on the strength, shape, and localization of the potentials.

Consider at $x_{\nu-1}<x<x_\nu$ a *currentless* wave function

$$\psi_c=\exp(G_\nu/2)\cos(kx-\phi_\nu/2) \ . \qquad (5)$$

A transmitted (to $x<x_1$) wave function

$$\exp(-ikx)=\cos(kx)-i\cos(kx-\pi/2)$$

corresponds to independent ψ_c^+ and ψ_c^- with $\phi_0=0$

and $\phi_0=\pi$, respectively. It generates the incident and reflected waves at $x > x_L$. Simple algebraic transformations determine the intensity transmission coefficient T and the dimensionless Landauer[6] resistance $R=T^{-1}-1$:

$$R=[\exp(G_L^+)+\exp(G_L^-)-2]/4 \ . \tag{6}$$

Applying θ_ν from Eq. (4) to ψ_c from Eq. (5), and defining $\omega_\nu, A_\nu, \rho_\nu$ by equations

$$\omega_\nu=\tan^2\left(\frac{\pi}{4}-h_\nu/2\right) \ , \quad \phi_\nu=2A_\nu+\beta_\nu+\gamma_\nu \ ,$$

$$\rho_\nu=(\gamma_\nu-\gamma_{\nu-1}-\beta_\nu-\beta_{\nu-1})/2 \ , \quad A_\nu-\rho_{\nu+1}=\tilde{\beta}_\nu \ ,$$

one obtains recurrence relations

$$\exp(G_\nu/2-iA_\nu)=\omega_\nu^{-1/2}\exp(G_{\nu-1}/2) \times(\cos\tilde{\beta}_{\nu-1}-i\omega_\nu\sin\tilde{\beta}_{\nu-1}) \ .$$

If $\tan A_\nu=X_\nu$, then, by the last equation,

$$X_\nu=\omega_\nu(X_{\nu-1}-r_\nu)/(1+r_\nu X_{\nu-1}); \ r_\nu=\tan\rho_\nu \ , \tag{7}$$

$$G_\nu=\sum_{n=1}^{\nu}\ln[(1+X_n^2)/(\omega_n+\omega_n^{-1}X_n^2)] \ ; \tag{8}$$

$$\exp(i\phi_\nu/2)=\sigma_{\nu-1}\exp[i(\beta_\nu+\gamma_\nu)/2] \times(1+iX_\mu)(1+X_\nu^2)^{-1/2} \ , \tag{9}$$

where $\sigma_\nu=\pm 1$ (and thus unimportant); $\sigma_\nu=\sigma_{\nu-1}\,\mathrm{sgn}[\cos\rho_{\nu+1}(1+r_{\nu+1}X_\nu)]$. If $\beta_0=0$, $\gamma_0=\pi/2$ [cf. Eq. (2)], then independent solutions correspond to

$$X_0=\tan(\phi_0/2-\pi/4)=\mp 1 \ .$$

In the case of the δ-function potentials (considered in Ref. 7), by Eq. (2),

$$r_\nu=\tan[ka_\nu-(h_\nu+h_{\nu-1})/2] \ .$$

Important implications follow directly from the obtained equations. In a random system at large (compared to the correlation length L_0) distances, the absence of the long-range order means that the terms in Eq. (8) "forget" the boundary conditions and become independent of each other and of the initial X_0 for any chain (numerical calculations verify it). Thus, in a single system, when $L\to\infty$, then $(G_L^+-G_L^-)\to$const, while $(G_L^++G_L^-)\propto L$ (and yields, together with $\ln R$, to the Gaussian distribution, in agreement with Ref. 8). Therefore, by Eq. (6),

$$R_L=[B_L\exp(G_L)-1]/2 \ ,$$

where

$$B_L=\cosh[(G_L^+-G_L^-)/2] \ , \quad G_L=(G_L^++G_L^-)/2 \ .$$

When $L\to\infty$, then in virtue of $G_L^+-G_L^-\to$const, $B_L\to$const, while $G_L/L\to 2/L_0$, where $L_0=\lim_{L\to\infty}(2L/\ln R)$ is the *wave-function* localization length. Since according to initial conditions, $G_0^+=G_0^-=0$, so $G_0=0$, $B_0=1$.

Simple calculations show that in the case of a weak scattering $\langle dA_L/dL\rangle_{L=0}\approx 2L/L_0$, where the angular brackets denote the ensemble averaging. So, $L\ll L_0$ implies $\langle R(L)\rangle\approx 2L/L_0$, and $L\gg L_0$ implies $\langle \ln R(L)>\simeq 2L/L_0$. This agrees with the scaling universality equation,[8] which can be presented as $\langle\ln(R+1)\rangle=2L/L_0$. When the scattering is strong, then the classical region is practically nonexistent, and this equation should also be valid. However, on a lattice ($x_\nu=\nu$) there exists a special case[9] ($k\simeq\pi$), when $L_0\gg 1$; B_∞ may be large; at $L\gg L_0$

$$\langle\ln R\rangle\simeq 2L/L_0+\ln(B_\infty/2) \ ; \tag{10}$$

$\langle\ln(R+1)\rangle$ is a complicated function of L at $L<L_0$, and its universality is violated. The obtained Eqs. (7)–(9) are very convenient for analytical as well as for numerical calculations, since they determine directly the exponent of the wave function. I consider Eq. (2) with $a_\nu=1$ and v_ν randomly chosen to be v (with the probability $c=0.5$) or zero (with the probability $c_1=1-c=0.5$). Figure 1 presents $\langle\ln(R+1)\rangle$ against the "universality variable" L/L_0. The averaging is performed over 10 000 random systems. Outside the immediate vicinity of $k=\pi$ when $L>1$, the argeement with the universality relation is remarkable—see $k=1.6$; $v=10$ and $v=0.3$. The dimensionless energy $k^2\simeq\pi^2\simeq 10$, so $v=10$ is an intermediate and $v=0.3$ is a weak potential. When k approaches π, the universality is invalidated. At $L>L_0$, $\langle\ln R\rangle$ yields to Eq. (10), where B_∞ increases when $(\pi-k)$ decreases. The results for other than in Fig. 1 v and c are similar. The region of the nonuniversality is $\pi-k\ll 1$, vc/π.

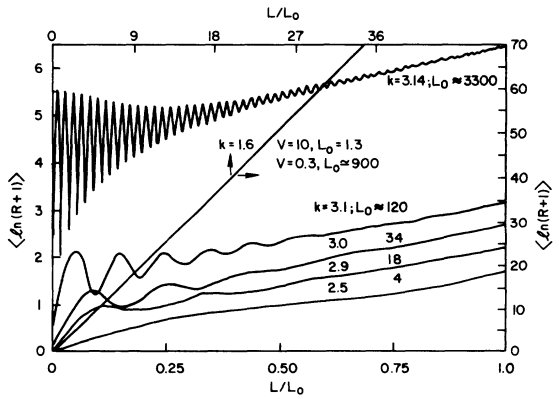

FIG. 1. The universality of the ensemble average of $\langle\ln(R+1)\rangle$, R is the resistance, for the wave vector $k=1.6$ and impurity concentration $c=0.5$. The nonuniversality of $\langle\ln(R+1)\rangle$ in the vicinity of $k\simeq\pi$ for $v=10$, $c=0.5$. All plots continue as straight lines for L/L_0 larger than in the figure.

III. ACOUSTIC PHONONS; LOCALIZATION AND EIGENSTATES

An harmonic chain with force constants λ_j, displacements $q_j \exp(-i\omega t)$, (t is time), and equal masses yields to the dimensionless equation,[4]

$$-\omega^2 q_j = \lambda_j(q_{j+1}-q_j)+\lambda_{j-1}(q_{j-1}-q_j) \ . \qquad (11)$$

[In the continuous case, when q_j, λ_j slowly change with j, Eq. (11) reduces to the equation for sound waves.] Introduce $\zeta_j=\lambda_j(q_{j+1}-q_j)$, $g_j=1-\lambda_j^{-1}$, and $\omega^2=2(1-\cos k)$, $|k|\leq\pi$. Then, by Eq. (11),

$$\zeta_{j+1}+\zeta_{j-1}-2\cos(k)\zeta_j=2(1-\cos k)g_j\zeta_j \ . \qquad (12)$$

Two real quantities $\zeta_{\nu-1}$, ζ_ν can be expressed through one complex "amplitude" δ_ν: $\zeta_j=\mathrm{Re}[\delta_\nu \exp(ikj)]$; $j=\nu, \nu+1$; a bar denotes the complex conjugation. By this equation, ζ_ν can be related to $\delta_{\nu-1}$ [if $j=(\nu-1)+1$] or to δ_ν (if $j=\nu$). This leads to the equation for $\delta_{\nu-1}$, δ_ν. Another relation between $\delta_{\nu-1}$ and δ_ν is provided by Eq. (12) with $j=\nu$. The two equations for complex $\delta_{\nu-1}$, δ_ν determine the recurrence from

$$\vec{\delta}_{\nu-1}=\begin{pmatrix}\delta_{\nu-1}\\ \bar{\delta}_{\nu-1}\end{pmatrix}$$

to $\vec{\delta}_\nu$ and thus from $\vec{\delta}_0$ to $\vec{\delta}_L$:

$$\vec{\delta}_L=\exp(-i\hat{k}L)\theta_L\theta_{L-1}\ldots\theta_1\vec{\delta}_0 \ .$$

Here $\hat{k}$ and θ_ν are the same as in Eqs. (3) and (4) with $h_\nu, \beta_\nu, \gamma_\nu$ from Eq. (2) and

$$a_\nu=1, \ v_\nu=2kg_\nu\tan(k/2) \ . \qquad (13)$$

Equation (13) maps the phonon problem[10] onto the extensively studied[8,11] problem of a particle in a random potential. Different masses in a harmonic chain are considered similarly; they just complicate the mapping equation. Now I demonstrate the approach (of the previous section) to the determination of the eigenstates. Figure 2(a) presents the "resistance" $R=T^{-1}-1$ for the wave $\zeta_j=\delta_\nu\exp(-ikj)$; g_ν in Eq. (13) is randomly chosen to be $g=0.9$ or 0 with equal probability $c=0.5$. The step in k is 0.001. The oscillations and the resonance minima of R at eigenvalues are pronounced. One of the minima is at $k=0.314$. Figure 2(b) presents $R(k)$ in the vicinity of this minimum on the blown-up scale, with the step in k equal to 10^{-7}. Note that the resonance at this eigenvalue ($k=0.3139650$, all digits are meaningful) has a half-width $\delta k \sim 2.10^{-6}$ and (see Fig. 2) leads to the decrease in R to $R=4.06$, i.e., by seven orders of magnitude. For this eigenvalue, the average relative amplitude of the displacments ζ_j is determined according to Eqs. (5)–(8) and (13) as a function of j and is presented in Fig. 3. It demonstrates a pronounced localization at $L\simeq 420$. The localization length $L_0\equiv\lim_{L\to\infty}(2L/\ln R)$ is in agreement with

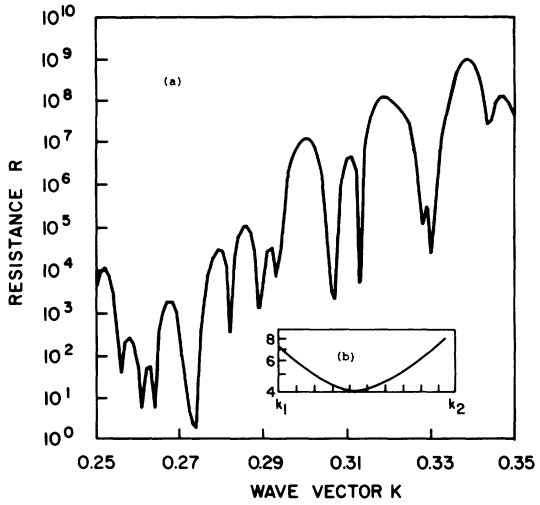

FIG. 2. Phonon resistance R against the wave vector k. The chain length $L=1000$; $k_1=0.313964$, $k_2=0.313966$.

the general formula[7] for $L_0(k)$, which in the case of $k \ll 1$ reads

$$L_0\simeq 8(1-gc)/[g^2c(1-c)k^2]\equiv \pi A/k^2 \ .$$

The detailed numerical analysis verifies the following general considerations. In the interval $k\sim\pi$ there are $\sim L$ randomly located eigenstates at the length L; thus, at the localization length L_0 there are $\sim L_0$ eigenvalues in the same interval of k. Therefore, a "local" characteristic distance Δk between eigenstates in $\Delta k \sim \pi/L_0$. This equation determines the characteristic local energy spectrum (and therefore the average local density of states) by a kind of the "Bohr

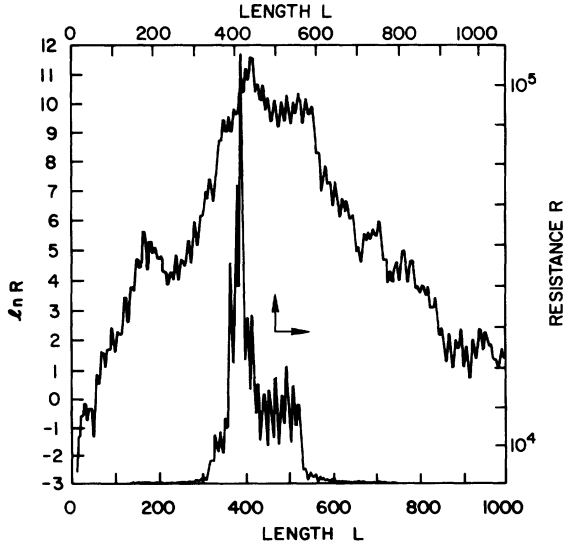

FIG. 3. The localization of the phonon eigenfunction on the regular and logarithmic scales.

quantization equation": $\int L_0 dk \sim n\pi$. The distance between the eigenstates, adjacent in their localization regions, is $\Delta k \sim \pi/L_0 \sim k^2/A$, and thus the nth local level has $k_n \sim A/n$; $L_0 \simeq \pi n^2/A$. So, the density of states increases with n. Of course, this spectrum is valid only until the localization length L_0 is less than the total length L. Since $k_n \leq k_{\max} \sim A$, when $g \gg 1$, the Debye temperature decreases $\propto 1/(1-c)g$.

IV. OTHER APPLICATIONS

The harmonic chain equation describes a number of other systems.[4] For instance, in the case of a diffusion, q_j in Eq. (11) is the Laplace transform of the density $\rho_j(t)$:

$$q_j = \int_0^\infty \rho_j(t) \exp(-\omega^2 t) dt \ ,$$

while λ_j is the hopping probability from the jth to the $(j+1)$st site. The same type of equation describes the Bloch electron in a magnetic field.[2] An electromagnetic wave in 1D also reduces to the Schrödinger-type equation: $E''(x) + \omega^2 \epsilon E = 0$, if $\mu = 1$; $H''(z) + \omega^2 \mu H = 0$, if $\epsilon = 1$, where electric E and magnetic H fields are perpendicular to x.

As an example, for thermodynamics, consider the Ising model with the Hamiltonian

$$\mathcal{H} = -\sum (J_j s_j s_{j-1} + H_j s_j); \ \ s_j = \pm 1 \ .$$

The partition function $Z_s^{(j)}$ for j sites with the spin s at the jth site yields to the equation

$$Z_s^{(j)} = \sum_{s'} \hat{\theta}_{ss'}^{(j)} Z_{s'}^{(j-1)} \ ,$$

where

$$\hat{\theta}_{ss'}^{(j)} = \exp(\tilde{J}_j s + \tilde{H}_j s') \equiv [2\sinh(2\tilde{J}_j)]^{1/2} \theta_{ss'}^{(j)} \ ,$$

$$\tilde{J}_j = J_j/T, \ \ \tilde{H}_j = H_j/T \ .$$

The matrix $\theta_{ss'}^{(j)}$ is the matrix from Eq. (4) with

$$h_j = \arcsin[\exp(-2\tilde{J}_j)] \ ; \ \ \gamma_j = \beta_j = -iH_j \ .$$

It leads to Eqs. (7)–(9) with the corresponding changes. For instance, one obtains the free energy

$$F_L \approx -\tilde{G}_L/2 + \sum_{j=1}^{L} \ln[2\sinh(2\tilde{J}_j)] \ .$$

Here

$$\tilde{G}_j = \sum \ln[(1-\tilde{X}_j^2)/(\tilde{\omega}_j - \tilde{\omega}_j^{-1}\tilde{X}_j^2)] \ ,$$

$$\tilde{X}_{j+1} = \tilde{\omega}_j(\tilde{X}_j + \tanh H_j)/(1 + \tilde{X}_j \tanh H_j)$$

and $\tilde{\omega}_j = \tanh J_j$. The spin correlation function $Q(L)$ at the distance L reduces to the ensemble average of $Z_{ss'}^{(j)}$, where s and s' are correspondingly the spins at the first and the $(L+1)$st sites.

Clearly, the application of the presented approach to different physical problems, listed in the Introduction, is straightforward in all cases (random, quasiperiodic and periodic with many atoms in a unit cell).

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