DOS and scattering matrix

Shell document for REVTEX 4.

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I. ONE-CHANNEL AND 1D - THESIS RESULT

We consider 1D system

$$-\frac{d^2\psi}{dx^2} + V(x)\psi = k^2\psi \tag{1}$$

closed at x = 0, i.e. $\psi(0) = 0$. In the scattering situation, a perfect lead is attached at x = L, Fig. 1, while for the closed system of length L, the corresponding boundary condition is imposed at x = L. For the scattering case, solution in the lead, x > L, is written as

$$\psi(x) = e^{-ik(x-L)} + e^{i\theta(k)}e^{ik(x-L)}, \ x \ge L.$$
(2)

The reflection delay time is defined as (??)

$$\tau(k) = \hbar \frac{d\theta(E)}{dE} = \frac{1}{v_g} \frac{d\theta(k)}{dk},\tag{3}$$

where $v_g = \hbar^{-1} \partial E / \partial k$ is the group velocity.

The joint probability distribution of the reflection phase $\tilde{\theta}$ and the delay time τ is

$$P(\theta,\tau) = \left\langle \delta\left(\tilde{\theta} - \theta\left(k\right)\right) \delta\left(\tau - \tau\left(k\right)\right) \right\rangle,\tag{4}$$

where $\theta(k)$ and $\tau(k)$ stand for the reflection phase and the delay time obtained for a given realization of disorder and energy $E = k^2$.



FIG. 1: Single-channel reflection from 1D system of length L.

First, we relate $\delta\left(\tilde{\theta} - \theta\left(k\right)\right)$ to the density of states inside the sample. Scattering solution $\psi(x)$ of the Schrödinger equation (1) satisfies boundary condition $\psi(0) = 0$, while at x = L it is matched to the solution in the lead, Eq. (2). Therefore, the logarithmic derivative of $\psi(x)$ satisfies

$$\frac{\psi'(L)}{\psi(L)} = k \tan \frac{\theta(k)}{2}.$$
(5)

On the other hand, with a fixed $\theta(k) = \tilde{\theta}$, Eq. (5) can be regarded as a second boundary condition for the solution inside the sample. Then, one obtains an eigenvalue problem on $x \in [0, L]$ with the boundary conditions

$$\psi(0) = 0, \ \frac{\psi'(L)}{\psi(L)} = k \tan\frac{\tilde{\theta}}{2} \tag{6}$$

(for example, $\tilde{\theta} = \pi$ corresponds to the Dirichlet BC at x = L). For this eigenvalue problem, density of states (DOS) per unit length

$$\nu_{\tilde{\theta}}(E) = \frac{1}{L} \sum_{\alpha} \delta(E - E_a), \qquad (7)$$

is related to the object $\delta\left(\tilde{\theta}-\theta\left(k\right)\right)$ as follows

$$\delta\left(\tilde{\theta} - \theta\left(E\right)\right) = \left(\frac{\partial\theta\left(k\right)}{\partial E}\right)^{-1} \sum_{\alpha} \delta\left(E - E_a\right) = \frac{L\nu_{\tilde{\theta}}\left(E\right)}{\tau\left(E\right)},\tag{8}$$

where definition (3) of the Wigner delay time, $\tau(E) = \frac{\partial \theta(E)}{\partial E}$, was used ($\hbar = 1$). Thus, DOS is related to the reflection phase and the delay time by

$$\nu_{\tilde{\theta}}\left(E\right) = \frac{1}{L}\tau\left(E\right)\delta\left(\tilde{\theta} - \theta\left(E\right)\right) \tag{9}$$

II. A RING WITH ONE SINGLE-CHANNEL LEAD

A. General

We consider here a simple system consisting of ring-shaped wire with one single channel lead attached to it, Fig. 2. This example was considered after Eric pointed out that DOS in the closed ring can be obtained from the delay time as

$$2\pi\rho_{ring}\left(E\right) = \lim_{\eta \to 0} \operatorname{Im} \frac{d}{dE} \ln \det S\left(E\right),\tag{10}$$

where S(E) is the scattering matrix (also for multiple lead case) and $\eta \in [0,1]$ is the coupling parameter ($\eta = 1$ corresponds to perfect coupling).

Below is a brief exercise checking explicitly the above statement.



FIG. 2: A ring wire with one single-channel lead. The lead coordinate x is set to zero at the connection point. The ring coordinate y is zero at the opposite point, changes clockwise and $y = \pm L/2$ at the connection point.

B. Description of the vertex

First, let us describe the boundary conditions on the lead connection point by the *vertex* scattering matrix [1]. Below two models are given, one for a completely symmetric and second for an asymmetric vertex.

1. A completely symmetric vertex

Here a symmetric vertex is described. Later on I have realized that this type of vertex is not appropriate for the present needs, since it can not describe the detachment of the lead form the ring, which should involve an asymmetry between the lead and the other legs of the vertex. However, description of the vertex has already been obtained and is given below. After it, the more relevant model is considered.

Thus, we assume that the (three-leg) vertex is symmetric and its time reversal invariant (TRI) energy independent scattering matrix is

$$s = \begin{pmatrix} r & t & t \\ t & r & t \\ t & t & r \end{pmatrix},\tag{11}$$

where r and t are the vertex reflection and the transmission amplitudes. Departing for a moment from the main notation of Fig. 2, the incident and out-coming waves in the vertex legs are e^{-ikx_i} and e^{ikx_i} respectively. Then, considering wave incident only from one lead and requiring the wavefunction continuity and the flux conservation one obtains

$$1 + r = t, \tag{12}$$

$$1 - |r|^2 = 2|t|^2, (13)$$

since in the lead of incidence the solution is $\sim (e^{-ikx_i} + re^{ikx_i})$. Actually, the same conditions are obtained from the unitarity property of the vertex scattering matrix, $ss^{\dagger} = \mathbf{I}$. Thus, we have four parameters for r and t and three equations (Eq. (12) has real and imaginary parts), which leaves a freedom for the choice of the reflection strength, i.e. for $R = |r|^2$ (note that for 3-leg vertex $|r| \neq 0$). We write $r = \sqrt{R}e^{i\phi}$ and from Eq. (12) obtain

$$1 + 2\sqrt{R}\cos\phi + R = \frac{1-R}{2},$$

i.e.

$$\cos\phi = -\frac{1+3R}{4\sqrt{R}}.\tag{14}$$

Thus, $\cos \phi < 0$, while the allowed values of R are obtained from $|\cos \phi| < 1$, which yields

$$R - \frac{4}{3}\sqrt{R} + \frac{1}{3} < 0$$

The equality holds for

$$\sqrt{R} = rac{2}{3} \pm \sqrt{rac{4}{9} - rac{1}{3}} = rac{2}{3} \pm rac{1}{3},$$

therefore

$$\frac{1}{3} \le \sqrt{R} \le 1. \tag{15}$$

As mentioned in the beginning of the present section, this completely symmetric vertex is inappropriate, since when the reflection into the lead tends to unity (a complete reflection), the same happens also inside the ring, i.e. the desired periodic boundary conditions in the ring are in fact replaced with the Dirichlet ones at the location of the vertex. This is not we wanted to obtain, which is taken care of below.

2. An asymmetric vertex

We need a model of the vertex allowing detachment of the lead, which leaves the unperturbed ring. This means that in the corresponding limit the reflection into lead tends to unity, while scattering of the wave inside the ring vanishes. Thus, there should be no symmetry between the lead and the other two legs belonging to the ring. The latter, of course can be assumed symmetric. Thus, the (TRI) vertex scattering matrix is

$$s = \begin{pmatrix} r & t & t \\ t & \rho & \tau \\ t & \tau & \rho \end{pmatrix}, \tag{16}$$

where the first index belong to the lead, while the other two (invariant in respect to their permutation) belong to the ring. Thus, the above scattering matrix is a symmetric unitary one with an additional symmetry in respect to permutation of the indices i = 2, 3. As discussed in the note II G below, Eq. (64), such matrix has (n = 3)

$$N_{sym}^{\{2|n\}} = \frac{1}{2}n\left(n-1\right) + 1 = 4,$$
(17)

independent real parameters, one of which is for the overall phase. In order to determine the explicit parametrization we use the unitarity condition, $ss^{\dagger} = I$, which yields equations

$$|r|^2 + 2|t|^2 = 1, (18)$$

$$tr^* + \rho t^* + \tau t^* = 0, (19)$$

$$|t|^{2} + |\rho|^{2} + |\tau|^{2} = 1,$$
(20)

$$|t|^2 + \tau \rho^* + \rho \tau^* = 0, \tag{21}$$

one of which, e.g. the first one, can be seen to be linearly dependent with the rest (namely, adding the last two gives

$$2|t|^{2} + |\rho + \tau|^{2} = 1,$$
(22)

substituting which into the second one, $(\rho + \tau) = -\frac{t}{t^*}r^*$, results in the first equation). Thus, we have $2 \times 4 - 4 = 4$ free real parameters, in accord with the above $N_{sym}^{\{2|n\}} = 4$. These four parameters still should comply to some unitary bounds, to be found from the above equation. In addition, the overall phase (one of the four parameters) can be fixed by some external condition, which we choose as the wavefunction continuity *inside* the ring (which does not, and must not, hold between the lead an the ring). Namely, subtracting (21) from (20) gives

$$\left|\rho - \tau\right|^2 = 1 \to \rho - \tau = e^{i\phi},\tag{23}$$

i.e. leaves the free phase, which can be fixed by the continuity condition inside the ring. The latter means

$$\rho - \tau = -1. \tag{24}$$

This can be obtained by considering the case of the wave incident only at one edge associated with the ring, e.g., $\psi_2(x_2) = (e^{-ikx_2} + \rho e^{ikx_2})$ and $\psi_3(x_3) = \tau e^{ikx_3}$, so that $\psi_2(0) = 1 + \rho = \tau = \psi_3(0)$.

Thus, fixing (24), we need to express ρ , r and t in terms of three (i.e., 4-1) free parameters, which are left to choose. Defining

$$r = \sqrt{R}e^{i\phi_r}, \ 0 \le R \le 1, \tag{25}$$

$$t = |t| e^{i\phi_t} = \sqrt{\frac{1-R}{2}} e^{i\phi_t},$$
(26)

by Eq. (18), and using (19) and (24), one obtains

$$\rho = -\frac{1 + \sqrt{R}e^{i\delta}}{2}, \ \delta = 2\phi_t - \phi_r.$$
(27)

In general, one can choose the free parameters as R, ϕ_r and δ . In the following it seems sufficient to consider the special simple case $\delta = \pi$, which gives

$$\rho = \frac{\sqrt{R} - 1}{2},\tag{28}$$

$$\tau = 1 + \rho = \frac{\sqrt{R} + 1}{2}.$$
(29)

$$\phi_t = \frac{\pi + \phi_r}{2} + \pi n \tag{30}$$

Thus, ρ vanishes and $\tau \to 1$ in the limit $R \to 0$, which is the desirable way of detachment of the lead from the ring. Finally, we have the following parametrization in terms of R and ϕ_r :

$$r = \sqrt{R}e^{i\phi_r}, \ 0 \le R \le 1, \ 0 \le \phi_r < 2\pi,$$

$$t = \pm i\sqrt{\frac{1-R}{2}}e^{i\phi_r/2},$$

$$\rho = \frac{\sqrt{R}-1}{2},$$

$$\tau = \frac{\sqrt{R}+1}{2}.$$
(31)

The special limiting cases are R = 0, 1, which give

$$\begin{split} R &= 0: \ r = 0, t = \pm i \frac{e^{i\phi_r/2}}{\sqrt{2}}, \rho = -\frac{1}{2}, \tau = \frac{1}{2}, \\ R &= 1: \ r = e^{i\phi_r}, t = 0, \rho = 0, \tau = 1, \end{split}$$

C. Scattering solution for the ring with a completely symmetric vertex

Solution inside the ring (Fig. 2) is

$$\psi_r\left(y\right) = \cos ky,$$

which is the only way to satisfy the continuity condition

$$\psi_r\left(y=-\frac{L}{2}\right)=\psi_r\left(y=\frac{L}{2}\right)$$

for the generic case of $kL \neq 2\pi n$. Solution in the lead is written as

$$\psi_l(x) = \frac{\cos(kL/2)}{\cos(\theta/2)}\cos\left(kx + \frac{\theta}{2}\right),$$

where θ is the reflection phase [for the scattering matrix S(E)]. Phase θ is found from the vertex boundary condition, defined by the vertex scattering matrix (11). Let's denote $x_1 = x$, $x_2 = y + L/2$ [for $y \to -L/2$] and $x_3 = -(y - L/2)$

[for $y \to L/2$]. Then

$$\psi_1(x_1) = \frac{\cos(kL/2)}{\cos(\theta/2)} \left[e^{-i\theta/2} e^{-ikx_1} + e^{i\theta/2} e^{ikx_1} \right],$$

$$\psi_2(x_2) = 2\cos k (x_2 - L/2) = e^{ikL/2} e^{-ikx_2} + e^{-ikL/2} e^{ikx_2},$$

$$\psi_3(x_3) = 2\cos k (L/2 - x_3) = e^{ikL/2} e^{-ikx_3} + e^{-ikL/2} e^{ikx_3},$$

which provides the incident and the outgoing amplitudes at the vertex. From the first raw in the vertex scattering matrix (11) we have

$$\frac{\cos\left(kL/2\right)}{\cos\left(\theta/2\right)}e^{i\theta/2} = r\frac{\cos\left(kL/2\right)}{\cos\left(\theta/2\right)}e^{-i\theta/2} + t\left[e^{ikL/2} + e^{ikL/2}\right],$$

which becomes, using Eq. (12),

$$\frac{e^{i\theta/2} - re^{-i\theta/2}}{\cos\frac{\theta}{2}} = 2t \left[\frac{\cos kL/2 + i\sin kL/2}{\cos (kL/2)} \right],$$

$$\frac{2\cos\frac{\theta}{2} - (1+r)e^{-i\theta/2}}{\cos\frac{\theta}{2}} = 2(1+r)\left[1 + i\tan\frac{kL}{2}\right],$$

$$2 - (1+r)\left[1 + i\tan\frac{\theta}{2}\right] = 2(1+r)\left[1 + i\tan\frac{kL}{2}\right].$$
(32)

Substituting $r = \sqrt{R}e^{i\phi}$ yields

$$2 - \left(1 + \sqrt{R}\left[\cos\phi + i\sin\phi\right]\right) \left[1 + i\tan\frac{\theta}{2}\right] = 2\left(1 + \sqrt{R}\left[\cos\phi + i\sin\phi\right]\right) \left[1 + i\tan\frac{kL}{2}\right],\tag{33}$$

the real and the imaginary parts of which are

Re:
$$2 - \left(1 + \sqrt{R}\cos\phi\right) + \sqrt{R}\sin\phi\tan\frac{\theta}{2} = 2\left(1 + \sqrt{R}\cos\phi\right) - 2\sqrt{R}\sin\phi\tan\frac{kL}{2},$$
 (34)

Im :
$$\left(1 + \sqrt{R}\cos\phi\right)\tan\frac{\theta}{2} + \sqrt{R}\sin\phi = 2\sqrt{R}\sin\phi + 2\left(1 + \sqrt{R}\cos\phi\right)\tan\frac{kL}{2}.$$
 (35)

The second one gives

$$\left(1 + \sqrt{R}\cos\phi\right)\left(\tan\frac{\theta}{2} - 2\tan\frac{kL}{2}\right) = \sqrt{R}\sin\phi,$$
$$\tan\frac{\theta}{2} = 2\tan\frac{kL}{2} + \frac{\sqrt{R}\sin\phi}{1 + \sqrt{R}\cos\phi}$$
(36)

From Eq. (14), and writing $\sin \phi = \pm \sqrt{1 - \cos^2 \phi}$, we obtain

$$\frac{\sqrt{R}\sin\phi}{1+\sqrt{R}\cos\phi} = \pm \frac{\sqrt{R}\sqrt{1-\cos^2\phi}}{1+\sqrt{R}\cos\phi} = \pm \frac{4}{3}\frac{\sqrt{R-\left(-\frac{1+3R}{4}\right)^2}}{1-R} = \pm \sqrt{\frac{R-\frac{1}{9}}{1-R}},\tag{37}$$

which gives finally the reflection phase in terms of k, L and the vertex reflection coefficient R:

$$\tan\frac{\theta}{2} = 2\tan\frac{kL}{2} \pm \sqrt{\frac{R - \frac{1}{9}}{1 - R}}.$$
(38)

Note that $\frac{1}{9} \leq R \leq 1$ according to Eq. (15), i.e. the additive term on the right hand side changes from zero to infinity as R increases from $\frac{1}{9}$ to 1. The lower value, $R = \frac{1}{9}$, corresponds to the "Neumann" boundary condition [1] on the vertex, i.e.

$$\sum_{i=1}^{3} \psi_i'(0) = 0. \tag{39}$$

It is convenient to introduce the coupling parameter

$$\eta = \frac{9}{8} \left(1 - R \right) \in [0, 1], \tag{40}$$

in terms of which Eq. (38) becomes

$$\tan\frac{\theta}{2} = 2\tan\frac{kL}{2} \pm \sqrt{\frac{1-\eta}{\eta}}.$$
(41)

D. Delay time and DOS - symmetric vertex

Now, using Eq. (41), we can calculate the delay time

$$\tau(E) = \frac{d\theta(E)}{dE}.$$
(42)

Differentiating Eq. (41) gives $(E = k^2 \text{ and } R \text{ is assumed independent of } E)$

$$\frac{d\theta}{dE} = \frac{L}{k} \frac{\cos^2 \frac{\theta}{2}}{\cos^2 \frac{kL}{2}}.$$
(43)

Using Eq. (41) and the identity

$$\frac{1}{\cos^2 \alpha} = 1 + \tan^2 \alpha,\tag{44}$$

yields

$$\tau_{\eta}\left(E\right) = \frac{d\theta}{dE} = \frac{L}{k} \frac{1 + \tan^2 \frac{kL}{2}}{1 + \left(2\tan\frac{kL}{2} \pm \sqrt{\frac{1-\eta}{\eta}}\right)^2}.$$
(45)

For "perfect" coupling, $\eta = 1$, the delay time is a smooth function

$$\tau_1(E) = \frac{L}{k} \frac{1 + \tan^2 \frac{kL}{2}}{1 + 4\tan^2 \frac{kL}{2}},\tag{46}$$

which has maxima at $kL = 2\pi n$, where $\tan^2 \frac{kL}{2} = 0$. For $\eta \to 0$, delay time $\tau_{\eta}(E)$ tends to a sum of δ -functions (this is not immediately evident from the above expression for $\tau_{\eta}(E)$, but becomes clear by considering $\theta(E)$ in Eq. 41, which behaves like a staircase in the limit $\eta \to 0$). The "problem" is that the location of the δ -functions is $kL = (2n+1)\pi$, i.e. not the resonant condition inside the ring. This is because the used above model for the vertex does not account for "clean" disconnecting of the lead from the ring, but rather for introducing a symmetric δ -function at the vertex in the limit $\eta \to 0$ (thus one has a ring with a δ -function, instead of a ring with a detached lead). In order to describe detachment of the lead, one needs to consider an antisymmetric vertex scattering matrix.

E. Scattering solution for the ring with an asymmetric vertex

Again, solution inside the ring (Fig. 2) is

$$\psi_r\left(y\right) = \cos ky,$$

which is the only way to satisfy the continuity condition

$$\psi_r\left(y = -\frac{L}{2}\right) = \psi_r\left(y = \frac{L}{2}\right)$$

for the generic case of $kL \neq 2\pi n$. Solution in the lead is written as

$$\psi_l(x) = A\cos\left(kx + \frac{\theta}{2}\right),$$

where θ is the reflection phase [for the scattering matrix S(E)] and A is some complex amplitude. There are three real parameters, A and θ , and we need three equations, obtained from the first two rows of the vertex scattering matrix (16). Let's denote $x_1 = x$, $x_2 = y + L/2$ [for $y \to -L/2$] and $x_3 = -(y - L/2)$ [for $y \to L/2$]. Then

$$\begin{split} \psi_1(x_1) &= A \left[e^{-i\theta/2} e^{-ikx_1} + e^{i\theta/2} e^{ikx_1} \right], \quad \text{[lead]} \\ \psi_2(x_2) &= 2\cos k \left(x_2 - L/2 \right) = e^{ikL/2} e^{-ikx_2} + e^{-ikL/2} e^{ikx_2}, \quad \text{[upper part of the ring]} \\ \psi_3(x_3) &= 2\cos k \left(L/2 - x_3 \right) = e^{ikL/2} e^{-ikx_3} + e^{-ikL/2} e^{ikx_3}, \quad \text{[lower part of the ring]} \end{split}$$

which provides the incident and the outgoing amplitudes at the vertex. From the first and second raws in the vertex scattering matrix (16) we have

$$Ae^{i\theta/2} = rAe^{-i\theta/2} + t \left[e^{ikL/2} + e^{ikL/2} \right],$$

$$e^{-ikL/2} = tAe^{-i\theta/2} + \rho e^{ikL/2} + \tau e^{ikL/2}.$$
 (47)

Eliminating the amplitude A,

$$A = \frac{e^{-ikL/2} - (\rho + \tau)e^{ikL/2}}{te^{-i\theta/2}},$$
(48)

one obtains an equation for the reflection phase θ :

$$\frac{e^{i\theta/2} - re^{-i\theta/2}}{e^{-i\theta/2}} = \frac{2t^2 e^{ikL/2}}{e^{-ikL/2} - (\rho + \tau) e^{ikL/2}},\tag{49}$$

which yields using Eq. (31)

$$S(E) = e^{i\theta} = r + \frac{2t^2}{e^{-ikL} - (\rho + \tau)} = \left[\sqrt{R} - \frac{1 - R}{e^{-ikL} - \sqrt{R}}\right] e^{i\phi_r} = \frac{\sqrt{R}e^{-iLk} - 1}{e^{-iLk} - \sqrt{R}}e^{i\phi_r}$$
(50)

F. Delay time and DOS - asymmetric vertex

From Eq. (50) one obtains the delay time $(v_g = dE/dk)$

τ

$$(E) = \frac{d\theta(E)}{dE} = \frac{1}{v_g} \frac{1}{ie^{i\theta}} \frac{de^{i\theta}}{dk} =$$

$$= \frac{1}{v_g} \frac{1}{i} \frac{\left(e^{-iLk} - \sqrt{R}\right)}{\sqrt{R}e^{-iLk} - 1} iL \frac{e^{-iLk}}{\left(e^{-iLk} - \sqrt{R}\right)^2} (R - 1)$$

$$= \frac{L}{v_g} \frac{1 - R}{\left(1 - \sqrt{R}e^{-iLk}\right) \left(1 - e^{iLk}\sqrt{R}\right)}$$

$$= \frac{L}{v_g} \frac{1 - R}{1 + R - 2\sqrt{R}\cos(Lk)}$$

$$= \frac{L}{v_g} \frac{\left(1 + \sqrt{R}\right) \left(1 - \sqrt{R}\right)}{\left(1 - \sqrt{R}\right)^2 + 4\sqrt{R}\sin^2\frac{Lk}{2}}.$$
(51)

In the limit $R \to 1$ this becomes (using $\int_{-\infty}^{\infty} \frac{1}{s^2+1} ds = \pi$)

$$\lim_{R \to 1} \tau\left(E\right) = \frac{2L}{v_g} \pi \delta\left(2\sin\frac{Lk}{2}\right) = 2\pi \frac{1}{v_g} \sum_{n=1}^{\infty} \delta\left(k - \frac{2\pi}{L}n\right).$$
(52)

This is *almost* the desired relation between the delay time and the DOS of the unperturbed ring

$$\rho_{ring}\left(E\right) = \frac{2}{v_g} \sum_{n=1}^{\infty} \delta\left(k - \frac{2\pi}{L}n\right).$$
(53)

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The problem is the missing factor of 2, which accounts for double degeneracy of the states in the ring (clockwise and counter-clockwise wave in the ring. Thus, Eq. (52) means $\lim_{R\to 1} \tau(E) = 2\pi \frac{\rho_{ring}(E)}{2}$. Assuming I have not done any mistake in the above calculations, the missing factor can be related to the fact that the translational invariance of the ring is removed for any finite (1 - R). This observation, however, is rather a hint for spotting the mistake than an explanation (since, by the Weyl expansion, DOS should be proportional to L with a standard factor). Note that I have made a shortcut and forced the symmetric solution inside the ring, $\cos ky$, while this constrain is not valid for exactly the eigenstate energies with $kL = 2\pi n$. Probably, defining the solution inside the ring in a general form $Ce^{iky} + Be^{-iky}$ is more careful and would restore the missing degeneracy factor. Alternativly, it may happen that careful consideration of the scattering solution near and at $kL = 2\pi n$ would show that the reflection phase should have a discontinuity of π as k crosses the values $k_n L = 2\pi n$.

G. Note: the number of the independent parameters of a unitary matrix with constrains

A unitary $n \times n$ matrix U satisfies

$$UU^{\dagger} = U^{\dagger}U = I, \tag{54}$$

which reduces a number of the independent *real* parameters from $2n^2$ (i.e. twice the number of the matrix elements) to n^2 . This can be obtained directly by counting the number of independent equations contained in Eq. (54). The detailed equations corresponding to the matrix equations in (54) are respectively

$$\sum_{k=1}^{n} u_{ik} u_{jk}^* = \delta_{ij}, \quad \sum_{k=1}^{n} u_{ki}^* u_{kj} = \delta_{ij}, \quad 1 \le i, j \le n,$$
(55)

which can be shown to be equivalent, i.e. by multiplying the first one by u_{ip}^* and summing over all i:

$$\sum_{i=1}^{n} u_{ip}^{*} \sum_{k=1}^{n} u_{ik} u_{jk}^{*} = \sum_{k=1}^{n} \left[\sum_{i=1}^{n} u_{ip}^{*} u_{ik} \right] u_{jk}^{*} = u_{jp}^{*} \rightarrow \sum_{i=1}^{n} u_{ip}^{*} u_{ik} = \delta_{pk},$$
(56)

that follows because $1 \le p, j \le n$ are arbitrary. Thus, we are left with only one of the sums in (55), say the first one, which is also symmetric in respect to the interchange of i and $j \left(\sum_{k=1}^{n} u_{jk} u_{ik}^* = \left[\sum_{k=1}^{n} u_{jk}^* u_{ik}\right]^* = \left[\sum_{k=1}^{n} u_{ik} u_{jk}^*\right]^* = \delta_{ij}$, therefore the independent equations are

$$\sum_{k=1}^{n} u_{ik} u_{jk}^* = \delta_{ij}, \quad 1 \le i \le j \le n,$$
(57)

which finally yields n^2 equation for the real parameters (*n* diagonal equations for the absolute values plus $2 \times \frac{n^2 - n}{2}$ off-diagonal equations. Finally, the number of the independent parameters for the general unitary matrix is

$$N_{gen} = 2n^2 - n^2 = n^2. (58)$$

This is an easily obtained result. Some difficulties arise, however, when additional constrains are added to the unitary matrix, such as symmetries. The problem is that the constrain equations can be partially dependent on the general equations given above, therefore the reduction of the number of the independent real parameters is not equal to the number of the added equations. The relevant for me constrains are symmetric unitary matrix $U = U^T$ (e.g. for the time reversal scattering matrix) and unitary matrix symmetric in respect to the interchange of some indices (i.e. symmetric in respect to the interchange of the scattering channels).

Let start from the symmetric unitary matrix $U = U^{T}$, which is the same as $U^{\dagger} = U^{*}$ (this is NOT an orthogonal matrix defined by $OO^{T} = I$). As mentioned above, it is difficult (at least for me) to count directly the total number of the independent equations. It is, however, becomes a simple task once one uses the representation of the unitary matrix in terms of the Hermitian one:

$$U = e^{iH}, \ H = H^{\dagger} \tag{59}$$

(an alternative useful representation is $U = \frac{I+iH}{I-iH}$).

First, one can find immediately a number of the independent real parameters for the general unitary matrix as a number of the parameters for the Hermitian matrix, i.e. n diagonal (real) parameters $(h_{ii} = h_{ii}^*)$ plus $2 \times \frac{n^2 - n}{2}$ parameters for the off-diagonal complex-valued elements, the total of n^2 real parameter, as found before, Eq. (58).

Next, let us add the symmetry constrain, $U = U^T$, which means

$$e^{iH} = \left[e^{iH}\right]^T = e^{iH^T} \rightarrow H = H^T \rightarrow H = H^*,$$

i.e. the Hermitian matrix H is real-valued. This gives the following number of real parameters (the off-diagonal elements now yield only one parameter instead of two):

$$N_{sym} = n + \frac{n^2 - n}{2} = \frac{1}{2}n(n+1), \qquad (60)$$

which is a result stated somewhere in the literature (for some reason I did not find the derivation...).

Finally, consider the symmetric unitary matrix with an additional symmetry of the interchange of some of the indices (some of the scattering channels). The transformation matrix for the interchange of two indices, say i = 1 and j = 2, is

$$Q_{12} = \begin{pmatrix} 0 & 1 & 0_{1 \times (n-2)} \\ 1 & 0 & 0_{1 \times (n-2)} \\ 0_{(n-2) \times 1} & 0_{(n-2) \times 1} & I_{(n-2) \times (n-2)} \end{pmatrix}, \ Q_{12} = Q_{12}^{\dagger}, \ Q_{12}Q_{12}^{\dagger} = I.$$
(61)

The interchange symmetry is

$$U = Q_{12}^{\dagger} U Q_{12} = Q_{12}^{\dagger} e^{iH} Q_{12} = \exp\left[iQ_{12}^{\dagger} H Q_{12}\right] \to Q_{12}^{\dagger} H Q_{12} = H,$$
(62)

i.e. the real Hermitian matrix H is also invariant under the index pair interchange. Thus, it remains to determine the number of the degrees of freedom reduced by this constrain. Matrices Q_{12} interchange the corresponding rows and columns, which gives $(h_{ij} = h_{ji})$

$$H = \begin{pmatrix} h_{11} & h_{12} & \cdots \\ h_{12} & h_{22} & \cdots \\ h_{1,j=\{\overline{3,n}\}} & h_{2,j=\{\overline{3,n}\}} & H_{(n-2)\times(n-2)} \end{pmatrix} = \begin{pmatrix} h_{22} & h_{12} & \cdots \\ h_{12} & h_{11} & \cdots \\ h_{2,j=\{\overline{3,n}\}} & h_{1,j=\{\overline{3,n}\}} & H_{(n-2)\times(n-2)} \end{pmatrix} = Q_{12}^{\dagger} H Q_{12}.$$
(63)

Thus, we have $h_{11} = h_{22}$ and (n-2) equations $h_{1,j=\{\overline{3,n}\}} = h_{2,j=\{\overline{3,n}\}}$, a total of (n-1) constrains. Therefore, a symmetric unitary matrix with an additional symmetry in respect to the interchange of a pair of indices (channels) has the following number of the independent real parameters

$$N_{sym}^{\{2|n\}} = N_{sym} - (n-1) = \frac{1}{2}n(n+1) - (n-1) = \frac{1}{2}n(n-1) + 1,$$
(64)

where the superscript $\{2|n\}$ means that two channels out of n are symmetric. To generalize this result to the case of m channels between them, note that in order to increase m by one we need to add only one symmetry transformation $Q_{m,(m+1)}$ (let us move all the symmetric channels to the lower indices). Then, generalizing Eq. (63) one sees that, for m > 2, adding m^{th} symmetric channel to (m-1) ones increases the number of the added constraints by 2 + (n-m). This is because we add one equation for the diagonal elements, (n-m) - for the interchanged column elements below the diagonal, and only one more for all the interchanged column elements above the diagonal (since these parts of the columns consist of identical elements). For example, for (m-1) = 3 one has

$$\begin{pmatrix} \rho & a & a \\ a & \rho & a \\ a & a & \rho \\ b & b & b \\ c & c & c \\ d & d & d \end{pmatrix} \begin{cases} b & c & d \\ b & c & d \\ b & c & d \\ f & s & e \\ g & e & t \end{pmatrix}$$

after adding m^{th} symmetric channel, the above diagonal part of the interchanged (m-1)'th and m'th column would only yield a single equation b = a. Thus, the total number of the additional constraints for m symmetric channels is

$$n_{eq}(m) = -1 + \sum_{k=2}^{m} 2 + (n-k) = -1 + (m-1)(2+n) - (m-1)\frac{m+2}{2} = (m-1)\frac{2n-m+2}{2} - 1, \quad (65)$$



FIG. 3: Construction of the triadic cantor set. The energies are the ends of the intervals remained at each iteration.

and the remaining number of the independent real parameters is

$$N_{sym}^{\{m|n\}} = N_{sym} - n_{eq}(m) = \frac{1}{2}n(n+1) - (m-1)\frac{2n-m+2}{2} + 1.$$
(66)

Note that this result corresponds to the case when there are $m \leq n$ channels symmetric between all of them. The case when there are more than one "invariant subspaces" seems to be different.

As an example, consider the complete symmetry between the channels, i.e. m = n, where one has

$$N_{sym}^{\{n|n\}} = \frac{1}{2}n\left(n+1\right) - \left(n-1\right)\frac{n+2}{2} + 1 = 2,\tag{67}$$

degrees of freedom, one of which corresponds to the overall phase of the matrix. Another example is the relevant case for the present context, i.e. n = 3 and m = 2, which gives

$$N_{sum}^{2-chan} (n=3) = 4, (68)$$

degrees of freedom, one of which is overall phase. This overall phase can be fixed by some physical considerations (e.g. wavefunction continuity at the scattering vertex).

III. HEAT KERNEL FOR CANTOR SET SPECTRUM (E.G., FOR FIBONACCI SUPERLATTICE)

A. Calculation of Z(t) for triadic Cantor set

We consider here the triadic Cantor, as defined in Eric's note (Fig. 3). One starts with an interval [0, 1], whose ends $\sigma_0 = \left\{\epsilon_0^{(0)} = 0, \epsilon_1^{(0)} = 1\right\}$ constitute the spectrum σ_0 at the iteration n = 0. At the first iteration, n = 1, the central third of the above interval is removed, so that the number of the ends is doubled and the spectrum becomes $\sigma_1 = \left\{\epsilon_0^{(0)} = 0, \epsilon_1^{(0)} = 1/3, \epsilon_2^{(0)} = 2/3, \epsilon_3^{(0)} = 1\right\}$. At the subsequent iterations each time the central third of the remaining intervals is removed and the number of the energies is doubled, while the obtained spectrum can be iterated self-similarly as follows

$$\sigma_n = \left\{ \epsilon_k^{(n)} \right\}_{k=0}^{k=2^{n+1}} \to \sigma_{n+1} = \left\{ \epsilon_k^{(n+1)} \right\}_{k=0}^{k=2^{n+2}} = \left\{ \frac{1}{3} \sigma_n \right\} \oplus \left\{ \frac{2}{3} + \frac{1}{3} \sigma_n \right\}.$$
(69)

Namely, at each new iteration the spectrum of the previous one is scaled by the scaling factor $l = \frac{1}{3}$ and copied twice with the left edge at 0 and $\frac{2}{3}$. This iterative relation gives a simple iterative relation between the heat kernels:

$$Z_{n+1}(t) = \sum_{k=0}^{2^{n+2}} e^{-\epsilon_k^{(n+1)}t} = \sum_{k=0}^{2^{n+1}} e^{-l\epsilon_k^{(n)}t} + \sum_{k=0}^{2^{n+1}} e^{-\left(2l+l\epsilon_k^{(n)}\right)t}$$
$$= \left(1+e^{-2lt}\right) \sum_{k=0}^{2^{n+1}} e^{-l\epsilon_k^{(n)}t} = \left(1+e^{-2lt}\right) Z_n\left(lt\right).$$
(70)

 \mathbf{n}

Then, iterating this expression down to n = 0, and using $Z_0(t) = 1 + e^{-t}$, one obtains

$$Z_n(t) = \left(1 + e^{-2lt}\right) \left(1 + e^{-2l^2t}\right) \left(1 + e^{-2l^3t}\right) \cdots \left(1 + e^{-2l^nt}\right) = \prod_{k=1}^n \left(1 + e^{-2l^kt}\right).$$
(71)

B. Sum over the bands

In optically commensurate photonic supelattice, i.e. where the optical path changes by a multiple of 2π in both layers when the wave number k is increamented by some Δ , the spectrum is repeated periodically in k with a period Δ (the energy, or frequency, is proportional to k, i.e. $\omega = kc$). If the introduced above σ_n represents one period of the whole spectrum, then the total heat kernel is sum over the periods of the spectrum:

$$Z_{tot}(t) = \sum_{p=0}^{\infty} \sum_{\sigma_n} e^{-(\epsilon_k + cp\Delta)t} = Z_n(t) \sum_{p=0}^{\infty} \sum_{\sigma_n} e^{-(cp\Delta)t} = \frac{Z_n(t)}{1 - e^{-(c\Delta)t}}.$$
(72)

C. Self-similar scaling relation for $Z_n(t)$

The general expression (71) yields the following scaling realtion for $Z_n(t)$

$$Z_n\left(\frac{t}{l}\right) = \prod_{k=1}^n \left(1 + e^{-2l^{(k-1)}t}\right) = \prod_{k'=0}^{n-1} \left(1 + e^{-2l^{k'}t}\right) = \frac{1 + e^{-2t}}{1 + e^{-2l^n t}} \prod_{k=1}^n \left(1 + e^{-2l^k t}\right)$$
(73)

i.e.

$$Z_n\left(\frac{t}{l}\right) = \frac{1+e^{-2t}}{1+e^{-2l^n t}} Z_n\left(t\right).$$

$$\tag{74}$$

In the limit of large n, i.e., $l^n t \ll 1$, this becomes

$$Z_n\left(\frac{t}{l}\right) = \frac{1+e^{-2t}}{2}Z_n\left(t\right).$$
(75)

For $1 \ll t \ll l^{-n}$, this further reduces to (the)

$$Z_n\left(\frac{t}{l}\right) = \frac{1}{2}Z_n\left(t\right). \tag{76}$$

Here the scaling factor $\frac{1}{2}$ is inverse to that in Eq. (2) of Eric's note, which seams to be correct, since $l = \frac{1}{3}$ and heat kernel should decrease with t. Function satisfying scaling (76) can be of the form $Z_n(t) = t^{-\alpha} f(\ln t)$ with $\alpha = -\ln 2/\ln l$ and periodic $f(x + \ln l) = f(x)$:

$$Z_n\left(\frac{t}{l}\right) = \left(\frac{t}{l}\right)^{-\alpha} f\left(\ln t - \ln l\right) = l^{\alpha} t^{-\alpha} f\left(\ln t\right) = \frac{1}{2} Z_n\left(t\right).$$

In the limit of small $t \ll 1$, scaling (75) becomes

$$Z_n\left(\frac{t}{l}\right) = \left[e^{-t} + O\left(t^2\right)\right] Z_n\left(t\right),\tag{77}$$

in agreement with the small-t approximation for Z(t) given in the next paragraph.

D. Small-*t* approximation for the heat kernel Z(t)

The small-t approximation for the heat kernel (71) can be obtained in different ways, one of which is the following

$$\begin{aligned} \ln Z_n\left(t\right) &= \ln \prod_{k=1}^n \left(1 + e^{-2l^k t}\right) = \sum_{k=1}^n \ln\left(1 + e^{-2l^k t}\right) \\ &= \sum_{k=1}^n \ln\left(2e^{-l^k t} \frac{e^{l^k t} + e^{-l^k t}}{2}\right) = n \ln 2 - t \sum_{k=1}^n l^k + \sum_{k=1}^n \ln\left(\frac{e^{l^k t} + e^{-l^k t}}{2}\right) \\ &= n \ln 2 - t \frac{l - l^n}{1 - l} + O\left(t^2\right),\end{aligned}$$



FIG. 4: Plot of $f(x) = \ln(1 + \exp[-2e^x])$.

which yields

$$Z_{n}(t) = 2^{n} \exp\left[-\frac{l-l^{n}}{1-l}t + O\left(t^{2}\right)\right].$$
(78)

In particular, for $\lim_{n\to\infty} l^n = 0$ and using $\frac{l}{1-l}\frac{1}{l} = \frac{l}{1-l}\frac{1-l+l}{l} = 1 + \frac{l-l^n}{1-l}$ we obtain

$$Z_n\left(\frac{t}{l}\right) = 2^n \exp\left[-\frac{l-l^n}{1-l}\frac{t}{l} + O\left(t^2\right)\right] = e^{-t}Z_n\left(t\right),\tag{79}$$

in agreement with (77).

E. Oscillations of heat kernel $Z_n(t)$

The oscillatory behaviour of $Z_n(t)$ takes place for $t \gtrsim 1$ (while $Z_n(t) \approx 2^n e^{-lt/(1-l)}$ for $t \ll 1$). This becomes evident by considering $\ln Z_n(t)$:

$$\ln Z_n(t) = \sum_{k=1}^n \ln \left(1 + \exp\left[-2e^{k\ln l + \ln t} \right] \right) = \sum_{k=1}^n f\left(k\ln l + \ln t\right), \tag{80}$$

where

$$f(x) = \ln(1 + \exp[-2e^x])$$
 (81)

plotted in Fig. 4. The sum in (80) is over the functions $f(k \ln l + \ln t)$ shifted by a multiple of $\ln l = -\ln 3$ along the axis $\ln t$, as shown in Fig. 5. Now it is clear that $W_n(y = \ln t) = \ln Z_n(t)$ has some periodic riples on the main decreasing background for $\ln 3 \leq \ln t \leq n \ln 3$. The background itself behaves like $\left(n - \frac{\ln t}{\ln 3}\right) \ln 2 + c$, where c is some constant of the order of unity (cf. Fig. 5). In order to write down this oscillations explicitly, one can use the Poisson summation formula

$$\sum_{k=-\infty}^{\infty} g\left(k\right) = \sum_{m=-\infty}^{\infty} \hat{g}\left(m\right); \ \hat{g}\left(m\right) = \int_{-\infty}^{\infty} g\left(k\right) e^{2\pi i m k} dk,$$
(82)

where the actual limits of summation over k are defined by the support of g(x). (Note: there is also a special case of the periodic summation formula,

$$\sum_{k=-\infty}^{\infty} g\left(x+kT\right) = \frac{1}{T} \sum_{m=-\infty}^{\infty} \hat{g}\left(\frac{m}{T}\right) \exp\left[2\pi i \frac{m}{T}x\right], \ \hat{g}\left(m\right) = \int_{-\infty}^{\infty} g\left(x\right) e^{2\pi i m x} dx,$$

which requires, however, the infinite summation over k).



FIG. 5: Visual representation of the sum in (80).

In our case we have, denoting $T = \ln l^{-1}$,

$$W_n(y) = \sum_{k=1}^n f(y - kT) = \frac{1}{2} \left[f(y - nT) - f(y) \right] + \sum_{m=-\infty}^\infty \int_0^n f(y - kT) e^{2\pi i mk} dk,$$

where for the convenience we have added and subtracted the k = 0 term, and the first term on the right hand side is required becouse of the exact limits of the integration in the integral on the RHS (the δ -functions implied in the Poisson summation are halved by these limits). Proceeding, one obtains

$$W_n(y) = \frac{1}{2} \left[f(y - nT) - f(y) \right] + \int_0^n f(y - kT) \, dk + 2 \sum_{m=1}^\infty \int_0^n f(y - kT) \cos(2\pi mk) \, dk$$
$$= \frac{f(y - nT) - f(y)}{2} + \frac{1}{T} \int_{y - nT}^y f(x) \, dx + \frac{T}{\pi m} \sum_{m=1}^\infty \int_0^n f'(y - kT) \sin(2\pi mk) \, dk,$$

where the intergation by parts was used for the oscillatory term. Let us consider separately the main non-oscillatory term and the rest oscillatory ones. Substituting the function f from Eq. (81) we have

$$W_n^{(bg)}(y) = \frac{f(y - nT) - f(y)}{2} + \frac{1}{T} \int_{y - nT}^y f(x) dx$$
$$= \frac{1}{2} \ln \frac{1 + \exp\left[-2e^{y - nT}\right]}{1 + \exp\left[-2e^y\right]} + \frac{1}{T} \int_{y - nT}^y \ln\left(1 + \exp\left[-2e^x\right]\right) dx.$$

This integral seems to be not expressible in elementary functions. Assuming that $y = \ln t \gg 1$ and $y - nT \ll -1$, we can rewrite it (semi-numerically) as

$$\int_{y-nT}^{y} \ln\left(1 + \exp\left[-2e^{x}\right]\right) dx = \int_{y-nT}^{-10} \ln\left(1 + \exp\left[-2e^{x}\right]\right) dx + \int_{-10}^{\infty} \ln\left(1 + \exp\left[-2e^{x}\right]\right) dx$$
$$\approx 6.2108377 + (nT - 10 - y) \ln 2,$$

where the number was obtained using numerical integration in Mathematica. Thus

$$W_n^{(bg)}(y) \approx \frac{1}{2} \ln \frac{1 + \exp\left[-2e^{y-nT}\right]}{1 + \exp\left[-2e^y\right]} + \frac{6.21084 + (nT - 10 - y)\ln 2}{T}$$
(83)

$$\approx \frac{6.2108377 - 10\ln 2}{T} + \left(n + \frac{1}{2} - \frac{y}{T}\right)\ln 2.$$
(84)

m	$\pi m a_m$	$\pi m b_m$
1	$9.7 imes 10^{-4}$	$-7.2 imes 10^{-4}$
2	$3.8 imes 10^{-8}$	$2.4 imes 10^{-7}$
3	$4.5 imes 10^{-8}$	-1.8×10^{-11}
4	$-2.7 imes10^{-9}$	4.1×10^{-15}
5	-1.5×10^{-9}	$2.5 imes 10^{-16}$

TABLE I: NUmerical values of the expansion coefficients a_m and b_m

The oscillatory terms are

$$W_n^{(osc)}(y) = \frac{T}{\pi m} \sum_{m=1}^{\infty} \int_0^n f'(y - kT) \sin(2\pi mk) \, dk =$$

= $\frac{T}{\pi m} \sum_{m=1}^{\infty} \int_0^n f'(y - kT) \sin(2\pi mk) \, dk$
= $\frac{1}{\pi m} \sum_{m=1}^{\infty} \int_{y - nT}^y f'(x) \sin\frac{2\pi m [y - x]}{T} \, dx$
= $-\frac{1}{\pi m} \sum_{m=1}^{\infty} \int_{y - nT}^y \frac{2e^x}{1 + \exp[2e^x]} \sin\frac{2\pi m [y - x]}{T} \, dx.$

Again, using the fact that f'(x) is peaked about zero, and assuming $y = \ln t \gg 1$ while $(y - nT) \ll -1$, one can extend to infinities the limits of the intergation in the last integral:

$$W_n^{(osc)}(y) = \frac{1}{\pi m} \sum_{m=1}^{\infty} \int_{-\infty}^{\infty} \frac{2e^x}{1 + \exp\left[2e^x\right]} \left[\cos\frac{2\pi my}{T} \sin\frac{2\pi mx}{T} - \cos\frac{2\pi mx}{T} \sin\frac{2\pi my}{T}\right] dx$$
(85)
$$= \sum_{m=1}^{\infty} a_m \cos\frac{2\pi my}{T} + b_m \sin\frac{2\pi my}{T},$$
(86)

where we have intruduced

$$\begin{cases} a_m \\ b_m \end{cases} = \frac{1}{\pi m} \int_{-\infty}^{\infty} \frac{2e^x}{1 + \exp\left[2e^x\right]} \begin{cases} \sin\frac{2\pi mx}{T} \\ -\cos\frac{2\pi mx}{T} \end{cases} dx.$$
 (87)

The intergrals a_m and b_m seem to be inexpressible analytically, and was calculated numerically for several values of m, as shown in Table I. Comparison of the numerical and the analytical results is given in Fig. 6.

T. Kottos and U. Smilansky, Quantum graphs: a simple model for chaotic scattering, J. Phys. A: Math. Gen. 36, 3501 (2003).



FIG. 6: Comparison of the numerical and the analytical results for W_{20} $(y = \ln t) = \ln Z_{20}(t)$. From the numerical sum (n = 20) the analytical expression for $W_{20}^{(bg)}(y)$ is extracted, and the remaining oscillatory term is compared to the analytical expression for $W_{20}^{(osc)}(y)$.