

## One-dimensional density of states and the phase of the transmission amplitude

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We derive a relationship between the one-dimensional density of states at energy  $E$  and the phase of the transmission amplitude at that energy by developing the two-channel  $S$ -matrix scattering theory for one-dimensional scattering and employing the relationship between traces of Green's-function operators and the on-shell  $S$  matrix.

The single-particle density of states is a central quantity in understanding many phenomena in a large number of physical systems. Interpretation of experimental spectra is in many cases directly tied to the density of states. The well-known algorithm for evaluating density of states,  $N(E)$ , is based on the trace of the Green's function  $G(E)$ ,  $N(E) = (2\pi)^{-1} \text{Im Tr} G(E)$ .<sup>1-3</sup> However the integral over the diagonal elements of the Green's function is often not simple to evaluate. Dashen, Ma, and Bernstein (DMB) related the trace of the Green's function, and therefore the density of states, to a quantity which is much simpler to calculate and relate to experiment, the on-shell  $S$  matrix  $S(E)$ .<sup>4</sup>

In some problems, one-dimensional models are of great utility in visualizing the physics of the phenomena under investigation. In particular, the one-dimensional density of states is of interest in many applications.<sup>2,3</sup> In order to use the DMB relation to calculate the one-dimensional density of states, the on-shell  $S$  matrix must be in hand. In this work we formulate one-dimensional scattering problems in the  $S$ -matrix language of formal scattering theory. After this is achieved, the derivation of the one-dimensional density of states is straightforward. We find that the density of states at energy  $E$ ,  $N(E)$ , is directly proportional to the derivative with respect to energy of the phase of the transmission amplitude  $t(E)$ . Unfortunately, our derivation cannot be generalized to obtain the local density of states in a restricted spatial (or momentum) coordinate region.<sup>3</sup>

It should be emphasized that our result is different from the well-known relationship between the density of states and the scattering phase shift in single-channel scattering problems, such as elastic scattering in a spherically symmetric potential.<sup>5</sup> In such problems the  $S$  matrix is a unimodular complex number, and its physical significance is the amplitude of the outgoing wave. The one-dimensional problem must be treated as a two-channel scattering problem (if no inelastic processes are considered), and the  $S$  matrix is a  $2 \times 2$  matrix. Thus, strange as it may seem, the  $S$ -matrix formulation of one-dimensional scattering problems is less trivial than single-channel scattering problems.

For simplicity, consider a one-dimensional potential  $V(x)$  which goes to zero as  $x$  goes to plus or minus infinity. We define channels 1 and 2 as waves traveling to the right and

left, respectively, and the channel states  $|m, k\rangle$ ,  $m = 1, 2$ :

$$\begin{aligned} |1, k\rangle &= \exp(ikx) , \\ |2, k\rangle &= \exp(-ikx) , \end{aligned} \quad (1)$$

where  $k = |\sqrt{2mE}|$ , and where atomic units are used. These states satisfy orthogonality and completeness. It is essential that the channel states be complete but not overcomplete, since only then can one define an  $S$  operator whose on-shell matrix elements  $\langle m, k | S | n, k \rangle = S_{m,n}(k)$  form a unitary  $2 \times 2$  matrix.<sup>6</sup> Here  $S_{m,n}(k)$  is the amplitude of the channel state  $|m, k\rangle$  after the interaction, assuming the state before the interaction is  $|n, k\rangle$ . With the use of these conventions for enumerating channels, it is evident that the  $S$ -matrix elements are related to the familiar transmission amplitudes  $t(E)$ , and reflection amplitudes from the left,  $r(E)$ , and from the right,  $r'(E)$ , namely,

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} t & r' \\ r & t \end{pmatrix} . \quad (2)$$

The transmission and reflection amplitudes are constrained by conservation of flux and time-reversal invariance

$$\begin{aligned} |t|^2 + |r|^2 &= |t|^2 + |r'|^2 = 1 , \\ t^*r + tr'^* &= 0 , \end{aligned} \quad (3)$$

which ensure the unitarity of the on-shell  $S$  matrix  $S_{m,n}(k)$ . Writing the quantities  $t, r, r'$  in terms of their magnitude and phases,

$$\begin{aligned} t &= |t|e^{i\theta} , \quad r = |r|e^{i\phi} , \\ r' &= |r| \exp\{i[2\theta - \phi + \pi(2m+1)]\} , \end{aligned} \quad (4)$$

and using the results of DMB, we can express the density of states in terms of the quantity  $d\theta/dE$ . We note in passing that the form of the  $S$  matrix appearing in Eq. (3) is different from the one used elsewhere.<sup>7</sup> Here  $S$  reduces to the unit matrix when the interaction is switched off. The  $S$  matrix defined in Eq. (3) is easily seen to be the on-shell restriction of the matrix elements of an  $S$  operator which is related to the  $T$  operator and the Green's function operator by the standard expressions of formal scattering theory, as we

shall now show. This is essential for implementation of the DMB algorithm.

Consider a one-dimensional scattering problem with Hamiltonian  $H = H_0 + V$ . We shall work in configuration space  $-\infty < x < \infty$  and for convenience use the same letter for an operator  $O$  and its representation  $\langle x|O|x' \rangle = O(x, x')$ . Thus

$$\langle x|H_0|x' \rangle = -\delta(x-x')d^2/dx^2$$

and for a local potential

$$\langle x|V|x' \rangle = \delta(x-x')V(x)$$

We now define the free Green's-function operator  $G_0(E) = (E - H_0)^{-1}$ , which in position representation takes the form

$$G_0(x, x'; E) = \langle x|G_0(E)|x' \rangle = \exp(ik|x-x'|)/2ik, \quad (5)$$

the full Green's-function operator  $G$ , and the  $T$  operator,

$$G = G_0 + G_0VG = G_0 + G_0TG_0, \quad (6)$$

$$T = V + VG_0T = V + VGV. \quad (7)$$

In what follows the energy dependence of  $G_0$ ,  $T$ , and  $G$  will sometimes be dropped. The  $T$  operator is easily related to the transmission and reflection amplitudes:

$$\begin{aligned} t &= 1 + (2ik)^{-1} \langle 1, k|T|1, k \rangle \\ &= 1 + (2ik)^{-1} \langle 2, k|T|2, k \rangle, \end{aligned} \quad (8)$$

$$\begin{aligned} r &= (2ik)^{-1} \langle 2, k|T|1, k \rangle, \\ r' &= (2ik)^{-1} \langle 1, k|T|2, k \rangle. \end{aligned}$$

To prove Eqs. (8), consider two solutions of the Schrödinger equation resulting from channel states traveling into the interaction region from the right and from the left,

$$\begin{aligned} |1, k \rangle &= |1, k \rangle + G_0V|1, k \rangle, \\ |2, k \rangle &= |2, k \rangle + G_0V|2, k \rangle. \end{aligned} \quad (9)$$

Using Eq. (6) and taking the limits as  $x$  goes to  $\infty$  and  $-\infty$ , we find<sup>8</sup>

$$|1, k \rangle \xrightarrow{x \rightarrow \infty} [1 + (2ik)^{-1} \langle 1, k|V|1, k \rangle]|1, k \rangle, \quad (10a)$$

$$|1, k \rangle \xrightarrow{x \rightarrow -\infty} |1, k \rangle + [(2ik)^{-1} \langle 2, k|V|1, k \rangle]|2, k \rangle. \quad (10b)$$

By definition, the quantities appearing in the square brackets are  $t$  and  $r$ . Substituting the integral equation (9) for  $|1, k \rangle$  into Eqs. (10) proves the first half of Eqs. (8). The second half of the proof is similar, starting from the asymptotic form of  $|2, k \rangle$ .

Now we define the  $S$  operator

$$S = 1 - 2\pi i\delta(E - H_0)T \quad (11)$$

and inspect its matrix elements in the momentum representation. On shell, it is easy to show that

$$\langle n, k|S|m, k \rangle = \delta_{n,m} + (2ik)^{-1} \langle n, k|T|m, k \rangle. \quad (12)$$

Hence, we have proved the existence of an  $S$  operator [de-

finied by Eq. (11)] whose on-shell matrix elements are the transmission and reflection amplitudes as asserted in Eq. (3).

Equipped with these identities we can now use the result of DMB:

$$-4i \operatorname{Im} \operatorname{Tr}[G(E) - G_0(E)] = \operatorname{Tr} \left[ S^{-1} \frac{dS}{dE} - \frac{dS^{-1}}{dE} S \right]. \quad (13)$$

An important step in DMB is the proof that Eq. (13) is true not only in operator form, but also that the right-hand side can be replaced by the on-shell  $S$  matrix, which in our case is given by Eq. (3). Since, on shell,  $S^{-1} = S^\dagger$ , we can use Eqs. (2) and (4) to evaluate the right-hand side of Eq. (13). The result is simply  $4i d\theta/dE$ . Thus, our final result is

$$\operatorname{Im} \operatorname{Tr}[G(E) - G_0(E)] = -d\theta/dE, \quad (14)$$

or

$$\pi[N(E) - N_0(E)] = d[\arg t(E)]/dE. \quad (15)$$

We should perhaps mention that the Hamiltonian  $H_0$  can contain a piece of the potential, and the proof here goes through unchanged, but the difference  $N - N_0$  represents the change in the density of states as a result of the additional potential  $H - H_0$ .

In conclusion, we compare the present method of calculation of one-dimensional density of states, and changes in the density of states due to a change in the potential, to other methods. The standard technique involves determination of the diagonal elements of the Green's function  $G(x, x; E)$ , and evaluation of the imaginary part of the trace  $\int dx G(x, x; E)$ .<sup>2,3</sup> Determination of  $G(x, x; E)$  for all  $x$  and the integration over  $x$  is much more involved than the determination of the transmission amplitude at energy  $E$  and at  $E + dE$ , from which  $d\theta/dE$  can be obtained. The method developed by Edwards and Beeby,<sup>9</sup> which can be used to calculate the density of states also for disordered systems, assumes that the potential is spherically symmetric within nonoverlapping spheres around each atom and constant between spheres. It is difficult to apply this method to determine the density of states due to the presence of a surface, or due to the addition of an adsorbed surface layer of adatoms. For the reduction of such surface problems to one-dimensional idealizations where only the coordinate normal to the surface is considered, the present method is vastly simpler. The method of Moliner and Rubio using factorization to obtain the Green's function for surface problems, and its generalization by Inglesfield and Velicky and Bartos has been used by a number of authors to study interface problems and electron structure of adatoms absorbed on metals.<sup>2</sup> Band and Efrim<sup>3</sup> generate the Green's function by a direct technique employing two linearly independent eigenfunctions at energy  $E$  with the appropriate boundary conditions at the two ends of the sample. Kalkstein and Soven<sup>10</sup> and Allan and Lenghart<sup>11</sup> used a Wannier-Bloch mixed representation to generate the Green's function for the surface of a cleave plane in the infinite crystal. Kambe<sup>12</sup> described a surface layer using Green's-function techniques. All of these methods are considerably more complicated than the present technique when applied to the one-dimensional idealization.

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