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Density of states and transmission in the one-dimensional scattering problem

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Abstract. From the analytic properties of transmission as a function of the complex wavevector we derive the dispersion relations connecting the transmission amplitude $|T(k)|$ and the change $\Delta\rho(k)$ in the density of states introduced by the scattering potential. We obtain several sum rules for both these quantities and we show that narrow resonances in $\Delta\rho(k)$ and in $|T(k)|^2$ have the same position and width.

The one-dimensional scattering problem has been studied mainly in relation to scattering by spherically symmetric potentials [1]. The inverse scattering problem i.e. how to find the potential from the scattering data, has also been considered for the purely one-dimensional case [2, 3]. This latter case differs from the radial Schrödinger equation not only in the absence of centrifugal potential $l(l+1)/r^2$ but also in the fact that the radial solutions exist only for $r \geqslant 0$ and are non-degenerate while the purely one-dimensional scattering involves twofold-degenerate functions defined for $x < 0$ and for $x \geqslant 0$. Recently, interest in this problem has revived owing to the studies of semiconductor heterostructures, e.g. resonant tunnelling diodes.

Two quantities have been frequently used to characterize the continuous spectra of one-dimensional structures: the transmission amplitude $|T(E)|$ and the density of states (DOS) $\rho(E)$. In fact, for an infinite system, $\rho(E)$ becomes infinite but its change $\Delta\rho(E) = \rho(E) - \rho_0(E)$ due to the scattering potential is finite for sufficiently localized potentials. In principle, $\Delta\rho(E)$ is a more universal quantity because it is well defined in cases when there is no transmission [4]. However, for the scattering on a bounded and localized potential the two quantities exist and have some similarities; in particular, for the double-barrier structure [4] the narrow resonances in $|T(E)|^2$ and in $\Delta\rho(E)$ have the same position and width. In the present paper we demonstrate the general relationships between $\Delta\rho(E)$ and $|T(E)|$ using the analytic properties of T studied as a function of the complex wavevector.

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We start from the relationship (obtained in [5] and rederived recently by ourselves [6]):

$$\Delta\rho(k) = (1/\pi)(\mathrm{d}\psi(k)/\mathrm{d}k) \tag{1}$$

where k is the wavevector ($E = \hbar^2 k^2/2m$) and $\psi(k)$ is the phase of the transmission coefficient $T(k) = |T(k)|\ \exp[\mathrm{i}\psi(k)]$. As was shown in [2], for the scattering potential $V(x)$ satisfying the condition

$$\int_{-\infty}^{+\infty} (1+|x|)|V(x)|\ \mathrm{d}x < \infty \tag{2}$$

the transmission coefficient $T(z)$ can be defined for the complex argument z and is a meromorphic function in the upper half-plane (Im $z \geqslant 0$). The only singularities in $T(z)$ in that region are simple poles on the imaginary axis ($z = \mathrm{i}\kappa_n$) corresponding to bound states in the potential $V(x)(|E_n| = (\hbar\kappa_n)^2/2m)$. On the real axis,

$$T(-k) = T^*(k). \tag{3}$$

Moreover, for $|z| \to \infty$, we have the asymptotic behaviour

$$T(z) \simeq 1 - \frac{\mathrm{i}\alpha}{z} \tag{4}$$

where

$$\alpha = \frac{m}{\hbar^2}\int_{-\infty}^{+\infty} V(x)\ \mathrm{d}x. \tag{5}$$

It can also be shown that the only zero of $T(z)$ for Im $z \geqslant 0$ can occur at $z = 0$ and it is then of first order. For the potential satisfying also the condition

$$\int_{-\infty}^{+\infty} x^2|V(x)|\ \mathrm{d}x < \infty \tag{6}$$

it can be shown that, for $|k| \to 0$,

$$T(k) \simeq -\mathrm{i}L_0 k(-1)^{N_b} \qquad L_0 > 0 \tag{7}$$

where N_b is the number of bound states of the potential. Applying to $T(z)$ the theorem giving the number N of zeros and number P of poles of a meromorphic function $f(z)$, i.e.

$$\frac{1}{2\pi\mathrm{i}}\oint \frac{f'(z)}{f(z)}\ \mathrm{d}z = N - P \tag{8}$$

and choosing the contour consisting of $[-R, -\epsilon]$ and $[\epsilon, R]$ on the real axis, the semicircle around zero of radius ϵ and the large semicircle of radius $R(R \to \infty, \epsilon \to 0)$, we obtain, for the transmission phase ψ,

$$\psi(R) - \psi(\epsilon) = \pi(\tfrac{1}{2} - N_b). \tag{9}$$

Therefore, if we choose, according to equation (7),

$$\psi(\epsilon) = \pi(N_b - \tfrac{1}{2}) \tag{10}$$

we obtain $\psi(\infty) = 0$, consistent with equation (4). Because of equation (3) we then have

$$\psi(-k) = -\psi(k) \tag{11}$$

so that $\psi(k)$ is continuous except at $k = 0$ where it jumps by $\pi(2N_b - 1)$. From equation (9) we obtain the sum rule for $\Delta\rho(k)$, namely

$$\int_{0_+}^{\infty} \Delta\rho(k)\ \mathrm{d}k = \tfrac{1}{2} - N_b \tag{12}$$

so that the bound states reduce the continuum DOS. It is interesting that for $N_b = 0$ (as for the double-barrier tunnelling structure) the total change in the continuum DOS is always $\frac{1}{2}$, even for the vanishingly small scattering potential. In this limit, $\Delta\rho(k) \to \delta(k)$. For the vanishingly small quantum well we always have a bound state ($N_b = 1$) and $\Delta\rho(k) \to -\delta(k)$.

In the lower half-plane we can also have simple poles of $T(z)$. If one such pole occurs near the real axis at $k_0 - \mathrm{i}\Gamma$, we have

$$T(z) \simeq \frac{T_0}{(z - k_0 + \mathrm{i}\Gamma)} \tag{13}$$

which gives, for real $z = k$,

$$|T(k)| \simeq \frac{|T_0|}{\sqrt{(k - k_0)^2 + \Gamma^2}}. \tag{14}$$

Thus we obtain a Lorentzian resonance of $|T(k)|^2$ centred at k_0 of width Γ. Knowing that $|T(k)| \leqslant 1$, we obtain $|T_0| \leqslant \Gamma$. The phase of $T(k)$ will be (ψ_0 is the phase of T_0)

$$\psi(k) \simeq \psi_0 - \tan^{-1}[\Gamma/(k - k_0)] \tag{15}$$

which gives, by virtue of equation (1),

$$\Delta\rho(k) \simeq \frac{1}{\pi}\frac{\Gamma}{(k - k_0)^2 + \Gamma^2}. \tag{16}$$

Thus the simple poles of $T(z)$ below the real axis give rise to Lorentzian resonances in $|T(k)|^2$ and in $\Delta\rho(k)$ with exactly the same position and width.

The general relationships between $\Delta\rho(k)$ and the transmission amplitude $|T(k)|$ can be obtained by considering the function $f(z)$

$$f(z) = \log\left(T(z)\frac{z+\mathrm{i}\beta}{z}\prod_{n=1}^{N_b}\frac{z-\mathrm{i}\kappa_n}{z+\kappa_n}\right) \tag{17}$$

analytic for $\mathrm{Im}\, z \geqslant 0$. The factor $(z+\mathrm{i}\beta)/z$ takes care of the zero of $T(z)$ when $|z| \to 0$. In the final results we take $\beta \to 0$. The remaining factors eliminate the poles for $z = \mathrm{i}\kappa_n$. For $|z| \to \infty$ the function $f(z)$ vanishes. Therefore we can obtain the standard dispersion relations [1] between the real and imaginary parts of $f(z)$. The first dispersion relation is

$$\begin{aligned}\log\left(|T(k)|\sqrt{1+\frac{\beta^2}{k^2}}\right) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\mathrm{d}k'}{k'-k}\Bigg[\psi(k') + \tan^{-1}\left(\frac{\beta}{k'}\right)\\ -2\sum_{n=1}^{N_b}\tan^{-1}\left(\frac{\kappa_n}{k'}\right)\Bigg]\end{aligned} \tag{18}$$

where $\mathcal{P}$ stands for the principal value of the integral. Using

$$\frac{1}{k'-k} = \frac{\mathrm{d}}{\mathrm{d}k'}\ \log(|k'-k|) \tag{19}$$

integrating by parts and setting $\beta \to 0$, we obtain

$$\log\left(\frac{|T(k)|}{k}\right) = -\frac{1}{\pi}\int_{-\infty}^{+\infty}\left(\frac{\mathrm{d}\psi(k')}{\mathrm{d}k'} + 2\sum_{n=1}^{N_b}\frac{\kappa_n}{k'^2+\kappa_n^2}\right)\ \log(|k'-k|). \tag{20}$$

Here we omit the principal value symbol because $\log|k'-k|$ is integrable around k. The integral of the second term in large parentheses can be performed analytically. After some simple transformations we obtain

$$\log\left[|T(k)|\prod_{n=1}^{N_b}\left(1+\frac{\kappa_n^2}{k^2}\right)\right] = -\int_{0_+}^{\infty}\mathrm{d}k'\ \Delta\rho(k')\ \log\left|1-\frac{k'^2}{k^2}\right|. \tag{21}$$

The lower integration limit is 0_+ which means that we avoid any $\delta(k')$ contributions to $\mathrm{d}\psi(k')/\mathrm{d}k'$ arising because of the discontinuity of $\psi(k')$ at zero. From the above formula we can obtain another sum rule for $\Delta\rho(k)$. For $|k| \to \infty$, according to equation (4),

$$\Delta\rho(k) \simeq \frac{\alpha}{\pi k^2} \tag{22}$$

while

$$|T(k)| \simeq 1 - \frac{\gamma}{k^2}. \tag{23}$$

Expanding $\log(1+\epsilon) \simeq \epsilon$ in equation (21), we obtain the sum rule

$$\sum_{n=1}^{N_b} \kappa_n^2 - \gamma = \int_{0_+}^{\infty} \mathrm{d}k'\ k'^2 \left(\Delta\rho(k') - \frac{\alpha}{\pi k'^2} \right). \tag{24}$$

Both terms in the large parentheses cannot be integrated separately but their difference is integrable. One could also differentiate both sides of equation (18) with respect to k, arriving at the dispersion relation which is the derivative of equation (21) but with the principal value of the integral.

Let us now turn to the second dispersion relation between the $\mathrm{Re}[f(z)]$ and $\mathrm{Im}[f(z)]$. Differentiating both sides with respect to k, we obtain (after some manipulations)

$$\Delta\rho(k) = -\frac{2}{\pi} \sum_{n=1}^{N_b} \frac{\kappa_n}{\kappa_n^2 + k^2} - \frac{1}{\pi^2} \mathcal{P} \int_0^{+\infty} \frac{k'}{k'^2 - k^2} \frac{\mathrm{d}}{\mathrm{d}k'} \{\log[|T(k')|^2]\}\ \mathrm{d}k' \tag{25}$$

where the terms containing β cancelled. We can see from equation (25) that each bound state reduces the DOS in the continuum by some quantity $\Delta\rho_n(k)$ with $\int_0^{+\infty} \Delta\rho_n(k)\ \mathrm{d}k = 1$. From the asymptotic behaviour of $\Delta\rho(k)$ (equation (22)) we can obtain from equation (25) the sum rule for the transmission amplitude:

$$\alpha + 2\sum_{n=1}^{N_b} \kappa_n = -\frac{1}{\pi} \int_0^{+\infty} \log|T(k')|^2\ \mathrm{d}k' \tag{26}$$

Let us finally note that the coincidence of narrow Lorentzian resonances in $\Delta\rho(k)$ and in $|T(k)|^2$ can be easily demonstrated using the dispersion relations (21) and (25).

Concluding, we have found general relationships between the transmission amplitude and the change in the DOS (equations (21) and (25)). We obtained two sum rules for $\Delta\rho(k)$ (equations (12) and (24)) and one sum rule for $|T(k)|^2$ (equation (26)). Narrow resonances in $\Delta\rho(k)$ correspond to simple poles of $T(z)$ slightly below the real axis and have the same position and width for $|T(k)|^2$ and $\Delta\rho(k)$.

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