Scaling behaviour of the transmission poles for Dirac comb

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The transmission poles of $N$ number of identical Dirac delta potentials placed periodically in one-dimension are examined in the complex-energy plane. The numerical results show that the imaginary part of the poles scales with $1/\sqrt{N}$. An approximate form of the poles is derived which supports the scaling behaviour of the poles found numerically. It is shown that the imaginary part of the poles are proportional to their real part for the poles close to the ends of the bands.

I. INTRODUCTION

In recent years, quantum transport in mesoscopic systems has become a rapidly developing research area\cite{1-4}. In the pioneering papers by Landauer and Büttiker it was shown that the conductance of such devices can be related to the transmission coefficients depending on the scattering properties of the system\cite{5-6}. In electron waveguide structures the resonant behaviour and the transmission phenomena have become an extensively studied problem\cite{7-8}. The transmission resonance caused by the quasi-bound states are in close connection with the poles of the transmission amplitude in the complex-energy plane. The quasi-bound state at energy $E_0$ and with decay time $\tau = \hbar/\Gamma$ corresponds to a simple pole in the transmission amplitude $t(z)$ at the complex-energy $z = E_0 - i\Gamma/2$ and the energy dependence of the transmission probability $T(E) = |t(E)|^2$ for $\Gamma \ll E_0$ is given by the well-known Breit-Wigner formula\cite{9,10}.

$$T(E) = \frac{\Gamma^2/4}{(E - E_0)^2 + \Gamma^2/4},$$

The pole structure of the transmission of a one-dimensional periodic array of Dirac delta potential (Dirac comb) is investigated in this paper. The transmission amplitude of $N$ unit cells is expressed by the transmission of one unit cell. The poles of the transmission amplitude are calculated numerically and a definite structure of the poles in the complex energy plane shows up. An analytical expression is derived for the imaginary part of the poles and it is shown that it scales with $N^{-1}$, where $N$ is the number of unit cells in the system. The agreement with the numerical results are excellent.

The rest of the paper is organised as follows. In section II using the transfer matrix method the transmission coefficient of $N$ number of unit cells is derived for the case of Dirac comb. In section III the numerical calculation of the poles are presented. In section IV an approximate expression of the poles are derived and compared with the numerical results. Finally, in section V our conclusions are given.

II. THE TRANSFER MATRIX APPROACH

In this section the transmission of an one-dimensional periodic array of $N$ Dirac delta potentials is considered. In one-dimension the single-channel description of the scattering process is valid. In this case Sprung et al.\cite{11} derived the following compact expression for the transfer matrix of $N$ number of periodically placed identical cells in terms of the 2x2 transfer matrix $M$ of a single-cell:

$$M^N = \frac{1}{\sin \Phi} [M \sin N\Phi - i \sin (N - 1)\Phi],$$

where $\cos \Phi = 1/2 \text{Tr}{} M$. Similarly, the following simple expression holds for the transmission probability $T_N = |t_N|^2$ of the $N$-cell array:

$$\frac{1}{|t_N|^2} = 1 + \frac{\sin^2 N\Phi}{\sin^2 \Phi} \left( \frac{1}{|t_1|^2} - 1 \right),$$

where $t_1$ is the transmission amplitude of a single-cell and the Bloch phase $\Phi$ associated with the infinite periodic potential is given by
\[
\cos \Phi = \text{Re}\left(1/t_1\right),
\]  
(4)

Note that the transmission amplitude depends on the energy of the electron involved in the scattering process.

These results can be applied for a one-dimensional periodic array of \(N\) Dirac-delta potentials. The transmission amplitude \(t_1\) for the case of unit cell containing a Dirac delta potential of strength \(\lambda\) and located in the centre of the unit cell is given by

\[
t_1 = \frac{k}{k + i\lambda/2}e^{ikd},
\]  
(5)

where \(k = \sqrt{E}\), the length of the unit cell is denoted by \(d\) and \(E\) is the energy of the electron. Hereafter we use the \(\hbar = 2m = 1\) units. Using Eq. (4) we find

\[
\cos \Phi(E) = \cos kd + \frac{\lambda}{2k} \sin kd.
\]  
(6)

The quasi-bound states of the system are given by the poles of the transmission amplitude in the complex energy plane. Hence, for the \(N\)-cell system \(1/T_N = 0\) which, using Eq. (5), can be written as

\[
1 + \frac{\sin^2 N\Phi}{\sin^2 \Phi} \left( \frac{1}{|T_1|^2} - 1 \right) = 0.
\]  
(7)

Thus, substituting Eq. (5) into the above equation one finds that for Dirac comb the complex energy \(E\) of the quasi-bound states is the solution of the following equation:

\[
-\frac{4E}{\lambda^2} = \frac{\sin^2 N\Phi(E)}{\sin^2 \Phi(E)}
\]  
(8)

where \(\Phi(E)\) is given by Eq. (6).

### III. NUMERICAL RESULTS

We now present the numerical solution of Eq. (8). In Fig. 1 the poles in the complex energy plane are shown for different number of Dirac delta potentials.

![FIG. 1. The poles of the transmission amplitude of the Dirac comb for \(N = 8, 16, 32\) number of Dirac deltas (the poles are denoted by plus signs, crosses and stars, respectively). The strength of the Dirac delta potentials, \(\lambda = 10.0\), and the distance between them, \(d = 4\).](image)
It can be seen that increasing the number of Dirac delta potentials, \( N \) in the array the poles move towards the real energy axis. It is also clear from the figure that the real part of the poles are separated into allowed and forbidden bands. The formation of the band structure of the infinite periodic array (Kronig-Penney model\(^2\)) can be seen even for \( N = 8 \). In each allowed band there are \( N - 1 \) number of poles. The width of the forbidden bands decreases with increasing the real part of the complex energy. The real part of the poles, \( E^m_l \) can be given by

\[
\Phi(E^m_l) = l\pi/N,
\]

where \( l = 1, \ldots N - 1 \) and \( \Phi(E) \) is given by Eq. (3). Hence, the real part of the \( l \)th poles in the \( m \)th band, \( E^m_l \) is determined by

\[
\cos k_l d + \frac{\lambda}{2k_l} \sin k_l d = \cos(l\pi/N),
\]

where \( k_l = \sqrt{E^m_l} \).

IV. SCALING OF THE POLES

In order to see the scaling behaviour of the poles an approximate solution of Eq. (8) for the quasi-bound states is derived.

The solution of Eq. (8) is a complex energy in the form of \( E = E^m_l - i\Gamma^m_l/2 \), where \( E^m_l \) is the \( N - 1 \) number of distinct solutions of Eq. (10) indexed by \( l \) in the \( m \)th allowed band and the decay time of the quasi-bound state is \( \hbar/\Gamma^m_l \). Assuming \( \Gamma^m_l/2 \ll E^m_l \), the Bloch phase \( \Phi(E) \) defined by Eq. (6), can be expanded in first order in \( \Gamma^m_l \) around \( E^m_l \):

\[
\Phi(E) \approx \Phi(E_0) + \delta\Phi(E^m_l, \Gamma^m_l),
\]

where

\[
\delta\Phi(E^m_l, \Gamma^m_l) = -i \frac{d\Phi(E)}{dE} \bigg|_{E^m_l} \frac{\Gamma^m_l}{2}.
\]

Finally, Eq. (8) becomes

\[
-\frac{4(E^m_l + i\Gamma^m_l/2)}{\lambda^2} = \frac{\sin^2 N(\Phi(E^m_l) + i\delta\Phi(E^m_l, \Gamma^m_l))}{\sin^2(\Phi(E^m_l) + i\delta\Phi(E^m_l, \Gamma^m_l))}.
\]

Substituting Eq. (4) into Eq. (13) and neglecting \( \delta\Phi \) in the denominator of the right hand side of Eq. (13) results in an implicit equation for \( \Gamma^m_l \) of the quasi-bound state:

\[
\frac{\Gamma^m_l}{2} = \frac{1}{N} \arcsinh \left( \frac{2\sqrt{E^m_l + i\Gamma^m_l/2} \sin (l\pi/N)}{\lambda} \right) \left( \frac{d\Phi(E)}{dE} \bigg|_{E^m_l} \right)^{-1},
\]

where the last factor can be determined from Eq. (6):

\[
\frac{d\Phi(E)}{dE} = \frac{d}{4k \sin \Phi} \left[ 2 + \frac{\lambda}{E d} \right] \sin k d - \frac{\lambda \cos kd}{k},
\]

and \( k = \sqrt{E} \). For \( \Gamma^m_l \ll E^m_l \) the implicit Eq. (14) can be solved iteratively for \( \Gamma^m_l \). Substituting \( \Gamma^m_l = 0 \) into the right hand side of Eq. (14) yields

\[
\frac{\Gamma^m_l}{2} = \frac{1}{N} \frac{4k_l \sin (l\pi/N)}{(\lambda k^2_l + 2d) \sin k_l d - (\lambda d/k_l) \cos k_l d} \arcsinh \left( \frac{2k_l \sin (l\pi/N)}{\lambda} \right).
\]

The approximate solution of Eq. (8) as the complex energy, \( E^m_l - i\Gamma^m_l/2 \) of the \( l \)th quasi-bound state in the \( m \)th band is given by Eqs. (13) and (14).
In Fig. 2 the numerically determined poles are shown for $N = 8, 16, 32$ number of Dirac delta potentials (this is an enlarged portion of Fig. 1) in the range of $66 \leq \text{Real}\{E\} \leq 75$ together with the approximate analytical solution given by Eqs. (10) and (16) when $E_l^m$ is taken as a continuous variable.

One can see that the envelope of the poles is well approximated by Eq. (16). The agreement between the analytic and the numerical solutions is excellent. Similar agreements are found in the other bands. The approximate solution becomes even better for increasing $N$. A small deviation appears only in the middle of the band but increasing $N$ it is decreasing. From Eq. (16) one can see that the imaginary part of the complex energy of the poles are proportional to $1/N$. It is easy to show that the factor multiplied by $1/N$ in Eq. (16) does not depend on $N$ in the leading order of $1/N$. Therefore, for large $N$ the imaginary part of the poles scales as

$$\Gamma_l^m \sim 1/N \quad (17)$$

for all the poles.

Using the numerical solutions of Eq. (8) in Fig. 3 $N\Gamma_l^m/2$ is plotted as a function of the real part of the poles for $N = 8, 16, 64$. As it is seen from the figure the numerically found poles follows the scaling behaviour of the poles given by Eq. (17). Again a very small deviation arises only at the middle of the bands for $N \leq 16$.

Using $\text{arsinh}(x) \approx x$ for $x \ll 1$ (in this case $\sin \Phi(E_l^m) \ll 1$) in Eq. (16) one can show that

$$\frac{\Gamma_l^m}{2} = E_l^m \lambda N \left(\frac{\lambda}{k_{lm}^2} + 2d\right) \frac{\sin^2(l\pi/N)}{(\lambda/k_{lm}) \sin k_{lm}d - (\lambda/k_{lm}) \cos k_{lm}d} \quad (18)$$
for fixed $N$ and $l \ll N$ or $N - l \ll N$ (these poles are close to the end of the band $m$). Again it can be shown that the factor multiplied by $E_{lm}^m$ in Eq. (18) is weakly dependent on the band index $m$ for those values of $E_{lm}^m$ when all the terms in the denominator of the right hand side of Eq. (15) is negligible except for the term $2d \sin k_{lm}d$. Thus, in the complex energy plane the poles at the end of each band move down from the real axis as the band index $m$ increases. This tendency can also be seen clearly from Fig. 1. However, from Eq. (18) a more rigorous statement can be made, namely at fixed $N$ and poles with $l$ close to the end of the band $\Gamma_{lm}^m \sim E_{lm}^m$. In Fig. 4 the imaginary part of the poles, $\Gamma_{lm}^m$ calculated numerically is plotted as a function of the real part of the poles, $E_{lm}^m$ for $l = 1$ as well as the analytic form given by Eq. (18).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure4.png}
\caption{\textit{\Gamma_{lm}^m/2 as a function of $E_{lm}^m$ for $N = 32$ and $l = 1$, and the plot of Eq. (18). The same parameters of the system are used as in Fig. 1.}}
\end{figure}

The numerically calculated poles are in good agreement with the analytic form given by Eq. (18) even for $N = 8$. The poles move down from the real axis in a way that their imaginary part are proportional to their real part for those poles which are close to the ends of the bands.

V. CONCLUSION

We have studied transmission properties of the one-dimensional periodic array of Dirac delta potential. Using the transfer matrix method a closed form of the transmission amplitude is given for finite number of Dirac delta potentials (finite number of unit cells in the Dirac comb). The quasi-bound states, which affect on the transmission properties of the system, are related to the poles of the transmission amplitude. The pole structure of the system is investigated for different number of unit cells in the Dirac comb.

The numerical solutions reveal a definite structure of the poles. The poles are well separated into allowed and forbidden bands much in the same way as in the Kronig-Penney model but the 'pole-spectrum' is not continuous. Each band contains $N - 1$ number of poles, where $N$ is the number of unit cells in the system. To check our numerical results an analytical form for the imaginary part of the poles has been derived. Although this is an approximate expression the comparison with the numerical results shows an excellent agreement especially for large $N$. From our analytic solution it has also been proved that the imaginary part of the poles is proportional to $1/N$. Furthermore, it has been demonstrated that for the poles close to the ends of the bands the imaginary part of the poles are again proportional to the real part of the poles.

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