The Finite Size Effect on Resonance Poles

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Abstract

The effect of the finite size of an array of scatterers on the position of the resonance poles of the scattered amplitudes is studied. This effect must be studied because in reality, an infinite array cannot be realized. In particular, it is expected that for a finite array of scatterers, the imaginary parts of the resonance poles (resonance widths) cannot vanish as is the case for an infinite double array admitting bound states in the radiation continuum.

1 Introduction

Let \( V_0(x, z) \) be a piecewise continuous function on the strip \( S = [-\frac{1}{2}, \frac{1}{2}] \times (-\infty, \infty) \) of an \( x, z \)-plane such that the support of \( V_0 \) is bounded. See Fig. 1(a) for a sketch. The potential \( V_0 \) represents a scatterer in the strip \( S \) for the scalar wave equation,

\[
\Delta E + k^2 V_0 E = -k^2 E
\]

Now, consider the following potentials obtained by translating the potential \( V_0 \) up and down the \( x \)-axis,

\[
V_N(x, z) = \sum_{n=-N}^{n=N} V_0(x-n, z), \quad V_\infty(x, z) = \sum_{n=-\infty}^{n=\infty} V_0(x-n, z)
\]

The potential \( V_\infty \) represents an infinite periodic array of period 1, while \( V_N \) represents its truncation to the first \( 2N+1 \) cells. See Fig. 1(b) for a sketch. Let \( E_N \) and \( E_\infty \) be solutions of the following wave equations,

\[
\Delta E_N + k^2 V_N E_N = -k^2 E_N, \quad \Delta E_\infty + k^2 V_\infty E_\infty = -k^2 E_\infty
\]

These solutions are both sought as the result of the scattering of an incident wave \( e^{ik\cdot r} \) by the potentials \( V_N \) and \( V_\infty \) respectively. In particular, they satisfy the Lippmann-Schwinger integral equations,

\[
E_N(r) = e^{ik\cdot r} + \frac{k^2}{4\pi} \int_{\mathbb{R}^2} V_N(r_0) E_N(r_0) G_k(r|\mathbf{r}_0) d\mathbf{r}_0
\]

where \( N \) is finite or infinite and \( G_k(r|\mathbf{r}_0) = i\pi H_0(k|r - \mathbf{r}_0|) \), where as usual, \( H_0 \) is the Hankel function of the first kind of zero order. It is important to point out that the sequence \( E_N \) cannot converge uniformly to \( E_\infty \). This is easily understood if one considers the behavior of \( E_N \) and \( E_\infty \) at the spatial infinity. For the field \( E_N \) when \( |\mathbf{r}| \rightarrow \infty \), then the scattered wave decays spherically since in the said limit \( E_N \rightarrow e^{ik\cdot r} + f(\theta)\frac{e^{ikr}}{\sqrt{r}} \)

where \( \theta \) is the polar angle between the position vector \( \mathbf{r} \) and the positive half of the \( x \)-axis in the \( x, z \)-plane, and \( f(\theta) \) is the scattered amplitude. On the contrary, for an infinite array, the solution \( E_\infty \) must satisfy Bloch’s periodicity condition in the \( x \)-direction, namely,

\[
E_\infty(x+1, z) = e^{ikx} E_\infty(x, z)
\]

Also, in the spatial infinity (\( |z| \rightarrow \infty \)), the wave fronts of the scattered wave \( E_\infty^\infty(r) = E_\infty(r) - e^{ik r} \) are planar, and perpendicular to the wave vectors of the open diffraction channels. Thus the convergence of \( E_N \) to \( E_\infty \) is at best pointwise. It follows that the asymptotics of \( E_N \) must be studied in a formalism that does not involve the spatial coordinates.
Figure 1: Panel (a): The potential $V_0$ represents a bounded scatterer in the strip $S = [-\frac{1}{2}, \frac{1}{2}] \times (-\infty, \infty)$ of the $x, z$-plane. The scatterer represented by $V_0$ need not be connected, it could be a collection of scatterers of different geometric shapes, and physical properties.

Panel (b): For the potential $V_N$, the scatterer represented by $V_0$ is shifted upwards and downwards by one unit to form $2N + 1$ identical scatterers. A periodic array of period one, and base scatterer $V_0$ is obtained in the limit $N \to \infty$.

2 T-matrix Formalism and Statement of the Results

Let the operators $\mathcal{F}_+$ and $\mathcal{F}_-$ denote the Fourier transform and inverse Fourier transform respectively, i.e.,

$$
\mathcal{F}_+[f](k) = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(r) e^{-ik \cdot r} \, dr, \quad \mathcal{F}_- [f](r) = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(k) e^{ik \cdot r} \, dk
$$

The $T$-matrix \[2\] of $E_N$ is,

$$
T_N = \mathcal{F}_+[V_N E_N] \tag{3}
$$

Let $S$ be the space of complex valued piecewise continuous functions on $\mathbb{R}^2$, and let $S'$ be the space,

$$
S' = \{G : \mathbb{R}^2 \to \mathbb{C} | \exists F \in S, G = \mathcal{F}_-[V_\infty F]\}
$$

Let then $\Omega_N$ be the operator defined by,

$$
\Omega_N[F] = \frac{k^2}{4\pi} \mathcal{F}_+[V_N] * (\mathcal{F}_+[G_k]F), \quad F \in S'
$$

In a similar fashion, we define an operator $\Omega_\infty$ on $S'$ by replacing $V_N$ in Eq.\[2\] by $V_\infty$.

By replacing $E_N$ in Eq.\[3\] by the right hand of Eq.\[1\], it is an easy exercise to see that $T_N$ satisfies the integral equation,

$$
T_N(K) = \Omega_N[T_N(E_N)] + D_N(K_x - k_x)Q(K - k) \tag{4}
$$

where $Q = \mathcal{F}_+[V_0]$, and $D_N$ is the Dirichlet kernel, i.e.,

$$
D_N(t) = \frac{\sin \left( (N + \frac{1}{2}) t \right)}{\sin \left( \frac{t}{2} \right)}
$$

In particular, in the limit $N \to \infty$, Eq.\[4\] must be understood in its distributional sense since the Dirichlet kernel converges to the Dirac comb,

$$
D_\infty(t) = 2\pi \sum_{m=-\infty}^{\infty} \delta(t - 2\pi m)
$$

Note also that in virtue of the Bloch’s condition \[2\], the $T$-matrix $T_\infty$ of $E_\infty$ is a distribution. Indeed,

$$
T_\infty(K) = \mathcal{F}_+[V_\infty E_\infty](K) = D_\infty(K_x - k_x)\mathcal{F}_+[V_0 E_\infty](K) \tag{5}
$$

The first step in studying the asymptotics of $T_N$ is decomposing $\Omega_N[T_N]$ as a sum of $\Omega_\infty[T_N]$ and a remainder. This is done by first observing that since $Q$ and $T_N$ are Fourier transforms of compactly supported functions, they extend to entire functions in their two variables. The following theorem then follows,
Theorem 1 (First Decomposition Theorem). Let $\mathcal{C}$ be the constant phase contour of the map $\theta \mapsto \cos(\theta)$ extending from $-\frac{\pi}{2} + i\infty$ to $\frac{\pi}{2} - i\infty$ through the saddle point 0 in the complex $\theta$-plane (See Fig. 2). Then,

$$ T_N(K) = \Omega_\infty [T_N](K) + R_N^+[T_N](K) + R_N^-[T_N](K) + D_N(K_x - k_x)Q(K - k) \quad (6) $$

where the remainders $R_N^\pm$ are defined by,

$$ R_N^\pm[T_N](K_x, K_z) = \frac{k^2}{2}\int_{\mathcal{C}} e^{i(N + \frac{1}{2})(k \cos(\theta) \pm K_z)} Q(K_x \pm k \cos(\theta), K_z - k \sin(\theta)) T_N(\mp k \cos(\theta), k \sin(\theta)) d\theta \quad \sin(\frac{1}{2}(k \cos(\theta) \pm K_z)) $$

Note that $\mathcal{C}$ is the usual steepest descent curve for the Hankel functions of the first kind [4].

![Figure 2: The contour of integration $\mathcal{C}$ for the remainders $R_N^+$ and $R_N^-$](image)

Figure 2: The contour of integration $\mathcal{C}$ for the remainders $R_N^+$ and $R_N^-$. It is the constant phase curve of the map $\theta \mapsto \cos(\theta)$ extending from $-\frac{\pi}{2} + i\infty$ to $\frac{\pi}{2} - i\infty$, and going through the saddle point at the origin of the $\theta$-plane.

Note that even though the remainders $R_N^\pm[T_N]$ are defined on steep descent curves for the map $\theta \mapsto \cos(\theta)$, the saddle point approximation [33] cannot be applied to get a first order approximation of the remainders. This is because $T_N$ is itself highly oscillatory as $N$ increases. Informally, one can understand this by observing that by the unicity of $E_N$, Eq. (6) can be inverted in the form,

$$ T_N = (1 - \Omega_\infty - R_N^- - R_N^-)^{-1} [\tau_k[D_N Q]] $$

where $\tau_k$ is the translation operator $\tau_k[F](K) = F(K - k)$. A first order correction should then be obtained from the Neumann series. However, this clearly fails since the action of $R_N$ on the highly oscillatory Dirichlet kernel $D_N$ will produce both highly oscillatory terms and terms that decay as $N \to \infty$. Therefore, $T_N$ must be decomposed into its oscillatory terms and converging terms. This is achieved by the following decomposition theorem.

Theorem 2 (Second Decomposition Theorem). Let $T_N^\pm(K)$ be the functions defined on $\mathbb{R}^2$ as,

$$ T_N^\pm(K) = Q(K - k) \frac{k^2}{4} e^{i(N + \frac{1}{2})k_x} \sin\left(\frac{1}{2}(K_x - k_x)\right) \times \int_{\mathcal{C}} e^{i(N + \frac{1}{2})k \cos(\theta)} Q(K_x \pm k \cos(\theta), K_z - k \sin(\theta)) T_N(\mp k \cos(\theta), k \sin(\theta)) d\theta \times \sin\left(\frac{1}{2}(k \cos(\theta) \pm K_z)\right) $$

And define $T_N^\pm$ and $T_N^\mp$ on $\mathbb{R}^2$ by,

$$ T_N^\pm = (1 - \Omega_\infty)^{-1}(T_N^+ + T_N^-), \quad T_N^\mp = (1 - \Omega_\infty)^{-1}(T_N^- - T_N^+) $$

Then, the map defined on $\mathbb{R}$ by $K_x \mapsto \frac{T_N^\pm(K_x, K_z)}{\sin\left(\frac{1}{2}(K_x - k_x)\right)}$ is continuous for all real $K_z$, and,

$$ T_N(K) = iD_N(K_x - k_x)T_N^\pm(K) + \cos\left(\frac{1}{2}(K_x - k_x)\right) \frac{T_N^\pm(K)}{\sin\left(\frac{1}{2}(K_x - k_x)\right)} \quad (7) $$

Furthermore, the sequences $\{T_N^\pm\}_{N=0}^\infty$ and $\{T_N^\mp\}_{N=0}^\infty$ converge uniformly to functions $T^\pm$ and $T^\mp$ respectively, where $T^\pm$ and $T^\mp$ extend analytically to the complex plane in both variables $K_x$ and $K_z$.

Thus the highly oscillatory terms in the $T$-matrix of the finite array are isolated from the converging terms. The oscillatory parts are given by the the Dirichlet kernel $D_N$ and the map $K_x \mapsto \cos\left(\frac{1}{2}(K_x - k_x)\right)$, while the converging terms are given by the maps $T_N^\pm$ and $T_N^\mp$. In particular, the solution $E_N$ of the Lippmann-Schwinger integral equation decomposes as follows,
Theorem 3. Let $T_N^i$, $i = 1, 2$ be defined as follows,
\[ T_N^i(K) = iD_N(K_x - k_x)T_N(K), \quad T_N^0(K) = \cos((N + \frac{1}{2})(K_x - k_x)) \frac{T_N(K)}{\sin(\frac{1}{2}(K_x - k_x))} \]

Then, $E_N(r) = e^{ikr} + E_N^1(r) + E_N^2(r)$ where $E_N^1 = F_-[F_+[G_k]T_N^0]$ and $E_N^2 = F_-[F_+[G_k]T_N^0]$. Moreover, $E_N^2$ converges uniformly to zero as $N \to \infty$ whereas $E_N^1$ converges pointwise to $E_N^2$.

**Proof.** The decomposition of $E_N$ follows from that of $T_N$ by first observing that if $E_i(r) = e^{ikr}$, then the Lippmann-Schwinger integral equation for $E_N$ can be rewritten as $E_N = E_i + G_k * (V_N E_N)$.

We then make use of the Fourier transform and its inverse as follows:
\[ G_k * (V_N E_N) = F_-[F_+[G_k]F_+(V_N E_N)] \]

By the definition of the $T$-matrix as given in Eq.(6), it follows that $E_N = E_i + F_-[F_+[G_k]T_N]$. Lastly, $T_N$ is replaced by its expression in $T_N^0$ and $T_N^2$ to obtain the decomposition of $E_N$.

That the sequence $\{E_N^2\}_{N=0}^\infty$ converges uniformly to zero follows from the Riemann-Lebesgue lemma. The pointwise convergence of $\{E_N^1\}_{N=0}^\infty$ to $E_\infty$ is a result of the convergence of the Dirichlet kernel to the Dirac comb.

Even though the decomposition of $T_\infty$ in Eq.(5) and the decomposition of $T_N$ in Eq.(7) suggest that $T_\infty^i(K) = F_+[V_0 E_\infty](K)$, this is not generally the case. The equality only holds necessarily when $K_x = k_x$, i.e., $T_\infty^i(k_x, K_z) = F_+[V_0 E_\infty](k_x, K_z)$ for all real $K_z$. From the meromorphic nature of the function $k^2 \mapsto E_\infty$ on the cut complex plane $\mathbb{C}_{k_x}$, follows the following theorem on the poles of the maps $k^2 \mapsto T_N^i$ and $T_N^2$:

**Theorem 4 (Asymptotic Behavior of the Poles).** For fixed $(k_x, K_z) \in \mathbb{R}^2$, the maps $k^2 \mapsto T_N^i(k^2; k_x, K_z)$ and $k^2 \mapsto T_N^2(k^2; k_x, K_z)$ extend meromorphically to the cut plane $\mathbb{C}_{k_x}$. If $E_\infty$ has a simple resonance pole $k^2 = \Gamma$, then so does $T_\infty^i(\cdot; k_x, K_z)$ and $T_N^i(\cdot; k_x, K_z)$ has a resonance pole $k_N^2 = \frac{1}{\sqrt{N}}$, $\Gamma_N = \Gamma + O(1/\sqrt{N})$ such that,

\[ k_N^2 = k_i^2 + O(\frac{1}{\sqrt{N}}), \quad \Gamma_N = \Gamma + O(\frac{1}{\sqrt{N}}) \]

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