Transfer matrix formulation of stationary scattering in two and three dimensional quantum mechanics

Farhang Loran

Isfahan University of Technology

Based on arXiv:2109.06528

12 November 2021

Overview

Scattering in $D = 1$

Consider a short-range potential in one dimension, $v : \mathbb{R} \to \mathbb{C}$, so that $|v(x)|$ tends to zero faster than $|x|^{-1}$ as $x \to \pm\infty$. Then, every solution of the stationary Schrödinger equation,

$$-\psi''(x) + v(x)\psi(x) = k^2\psi(x) \qquad x \in \mathbb{R},$$

satisfies

$$\psi(x) \to \begin{cases} A_- e^{ikx} + B_- e^{-ikx} & \text{for} \quad x \to -\infty, \\ A_+ e^{ikx} + B_+ e^{-ikx} & \text{for} \quad x \to +\infty, \end{cases}$$

Transfer Matrix

$A_\pm$ and $B_\pm$ are complex coefficients. The transfer matrix of the potential v is a 2×2 matrix $\mathbf{M}$ that relates (A_+, B_+) to (A_-, B_-) according to

$$\begin{bmatrix} A_+ \\ B_+ \end{bmatrix} = \mathbf{M} \begin{bmatrix} A_- \\ B_- \end{bmatrix}.$$

Composition rule

If we divide $\mathbb{R}$ into n adjacent intervals of the form,

$$I_1 := (-\infty, a_1), \quad I_2 := [a_1, a_2), \quad \cdots \quad I_n := [a_{n-1}, \infty),$$

such that $a_1 < a_2 < \cdots < a_{n-1}$, let $v_j : \mathbb{R} \to \mathbb{C}$ be the truncation of v given by

$$v_j(x) := \begin{cases} v(x) & \text{for} \quad x \in I_j, \\ 0 & \text{for} \quad x \notin I_j, \end{cases}$$

and $\mathbf{M}_j$ be the transfer matrix of v_j, then the following composition rule holds

$$\mathbf{M} = \mathbf{M}_n \mathbf{M}_{n-1} \cdots \mathbf{M}_1. \tag{1}$$

Dynamical formulation of stationary scattering

These results can be obtained by using the dynamical formulation of stationary scattering in one dimension. In this approach **M** is identified with the S-matrix of an effective non-unitary two-level quantum system.

A. Mostafazadeh, "A Dynamical formulation of one-dimensional scattering theory and its applications in optics," Ann. Phys. (N.Y.) **341**, 77 (2014).

A. Mostafazadeh, "Transfer matrices as non-unitary S-matrices, multimode unidirectional invisibility, and perturbative inverse scattering," Phys. Rev. A **89**, 012709 (2014).

Let ψ be the general bounded solution ψ of the stationary Schrödinger equation, and define

$$\big(\Psi_\pm(x)\big)(p) := \frac{1}{2k}\, e^{\pm ikx}\, \big[k\psi(x) \pm i\,\psi'(x)\big], \quad \mathbf{\Psi}(x) := \begin{bmatrix} \Psi_-(x) \\ \Psi_+(x) \end{bmatrix},$$

The stationary Schrödinger equation reads

$$i\partial_x \mathbf{\Psi}(x) = \widehat{\mathbf{H}}(x)\mathbf{\Psi}(x), \qquad \widehat{\mathbf{H}}(x) := \frac{v(x)}{2k} e^{-ikx\sigma_3} \boldsymbol{\mathcal{K}}\, e^{ikx\sigma_3}$$

where σ_3 is the diagonal Pauli matrix and

$$\boldsymbol{\mathcal{K}} := \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix},$$

We realize that

$$\lim_{x\to\infty} \mathbf{\Psi}(x) = \begin{bmatrix} A_+ \\ B_+ \end{bmatrix} \quad \lim_{x\to-\infty} \mathbf{\Psi}(x) = \begin{bmatrix} A_- \\ B_- \end{bmatrix}$$

and

$$\mathbf{M} = \mathscr{T} \exp\left[-i \int_{-\infty}^{\infty} dx\, \widehat{\mathbf{H}}(x)\right],$$

where $\mathscr{T}$ denotes the time-ordering operation with x playing the role of "time."

Dynamical equation for transfer matrix in higher dimensions

Adopt a coordinate system in which the source of the incident wave and the detectors used to observe the scattered wave lie on the planes $x = \pm\infty$.
Consider the stationary Schrödinger equation in $D + 1$ dimensions,

$$[-\partial_x^2 - \nabla^2 + v(x, \mathbf{y})]\psi(x, \mathbf{y}) = k^2\psi(x, \mathbf{y}), \qquad (x, \mathbf{y}) \in \mathbb{R}^{D+1},$$

for a short-range potential $v : \mathbb{R}^{D+1} \to \mathbb{C}$ and a wavenumber $k \in \mathbb{R}^+$. ∇^2 stands for the D-dimensional Laplacian.

Performing the Fourier transform of both sides of the Schrödinger equation with respect to $\mathbf{y}$, we find

$$-\tilde{\psi}''(x,\mathbf{p})+(\widehat{\mathscr{V}}(x)\tilde{\psi})(x,\mathbf{p}) = \varpi(\mathbf{p})^2\,\tilde{\psi}(x,\mathbf{p}), \qquad (x,\mathbf{p})\in\mathbb{R}^{D+1},$$

where a prime stands for differentiation with respect to x, $\tilde{\psi}(x,\mathbf{p}) := \mathcal{F}_{y,\mathbf{p}}\{\psi(x,\mathbf{y})\}$,

$$(\widehat{\mathscr{V}}(x)\tilde{f})(\mathbf{p}) := \mathcal{F}_{\mathbf{y},\mathbf{p}}\{v(x,\mathbf{y})f(\mathbf{y})\} = \frac{1}{(2\pi)^D}\int d^Dq\,\tilde{v}(x,\mathbf{p}-\mathbf{q})\tilde{f}(\mathbf{q}),$$

and

$$\varpi(\mathbf{p}) := \begin{cases} \sqrt{k^2-\mathbf{p}^2} & \text{for} \quad |\mathbf{p}|<k, \\ i\sqrt{\mathbf{p}^2-k^2} & \text{for} \quad |\mathbf{p}|\geq k. \end{cases}$$

We confine our attention to the class of potentials whose supports along the x-axis is finite, i.e, , we suppose that there are real numbers $a_\pm$ such that $a_- < a_+$ and

$$v(x,\mathbf{y}) = 0 \quad \text{for} \quad x \notin [a_-, a_+].$$

Then, $\tilde{v}(x,\mathbf{p}) = 0$ for $x \notin [a_-, a_+]$, and we obtain

$$[\partial_x^2 + \varpi(\mathbf{p})^2]\tilde{\psi}(x,p) = 0 \quad \text{for} \quad x \notin [a_-, a_+].$$

$$\tilde{\psi}(x,\mathbf{p}) \quad = \quad \begin{cases} A_-(\mathbf{p})e^{i\varpi(\mathbf{p})x} + \mathscr{B}_-(\mathbf{p})e^{-i\varpi(\mathbf{p})x} & \text{for} \quad x \le a_-, \\ \mathscr{A}_+(\mathbf{p})e^{i\varpi(\mathbf{p})x} + B_+(\mathbf{p})e^{-i\varpi(\mathbf{p})x} & \text{for} \quad x \ge a_+. \end{cases}$$

$$\begin{bmatrix} \mathscr{A}_+ \\ B_+ \end{bmatrix} = \hat{\mathfrak{M}} \begin{bmatrix} A_- \\ \mathscr{B}_- \end{bmatrix}.$$

Auxiliary transfer matrix

$$(\Phi_\pm(x))(\mathbf{p}) := \frac{e^{\pm i\varpi(\mathbf{p})x}}{2\varpi(\mathbf{p})}\left[\varpi(\mathbf{p})\tilde{\psi}(x,\mathbf{p}) \pm i\,\tilde{\psi}'(x,\mathbf{p})\right],$$

$$\boldsymbol{\Phi}(x) := \left[\begin{array}{c} \Phi_-(x) \\ \Phi_+(x) \end{array}\right],$$

The Schrödinger equation reads

$$i\partial_x \mathbf{\Phi}(x) = \widehat{\boldsymbol{\mathcal{H}}}(x)\mathbf{\Phi}(x)$$

in which

$$\widehat{\boldsymbol{\mathcal{H}}}(x) \quad := \quad \frac{1}{2}\varpi(\hat{p})^{-1}\, e^{-i\varpi(\hat{p})x\sigma_3}\,\widehat{\mathscr{V}}(x)\,\boldsymbol{\mathcal{K}}\, e^{i\varpi(\hat{p})x\sigma_3}.$$

Recall $\boldsymbol{\mathcal{K}} := \sigma_3 + i\sigma_2$ and

$$(\widehat{\mathscr{V}}(x)\tilde{f})(\mathbf{p}) = \frac{1}{(2\pi)^D}\int d^D q\,\tilde{v}(x, \mathbf{p}-\mathbf{q})\tilde{f}(\mathbf{q}),$$

$$\lim_{x\to-\infty}\mathbf{\Phi}(x)=\mathbf{\Phi}(a_-)=\begin{bmatrix} A_- \\ \mathscr{B}_- \end{bmatrix},\quad \lim_{x\to+\infty}\mathbf{\Phi}(x)=\mathbf{\Phi}(a_+)=\begin{bmatrix} \mathscr{A}_+ \\ B_+ \end{bmatrix}.$$

Thus

$$\hat{\mathfrak{M}}=\mathscr{T}\exp\left[-i\int_{-\infty}^{\infty}dx\,\widehat{\boldsymbol{\mathcal{H}}}(x)\right],$$

Composition rule for the auxiliary transfer matrix

Let ℓ be a positive integer, and $a_0, a_1, a_2, \cdots, a_\ell$ are arbitrary real numbers such that

$$a_- = a_0 < a_1 < a_2 < \cdots < a_{\ell-1} < a_\ell = a_+,$$

and $v_j : \mathbb{R} \to \mathbb{C}$ be truncations of the potential v given by

$$v_{m+1}(x,y) := \begin{cases} v(x,y) & \text{for} \quad x \in (a_m, a_{m+1}], \\ 0 & \text{for} \quad x \notin (a_m, a_{m+1}], \end{cases}$$

with $m \in \{0, 1, \cdots, \ell-1\}$. Let $\hat{\mathfrak{M}}_j$ be the analogs of $\hat{\mathfrak{M}}$ for the potentials v_j. Then,

$$\hat{\mathfrak{M}} = \hat{\mathfrak{M}}_\ell \hat{\mathfrak{M}}_{\ell-1} \cdots \hat{\mathfrak{M}}_1.$$

Perfect broadband invisibility

The omnidirectional invisibility for a wavenumber k corresponds to the requirement that, for this particular value of k, the restriction of $\hat{\mathfrak{M}}$ to the subspace of asymptotically oscillating modes equals the corresponding identity operator:

$$\widehat{\mathbf{\Pi}}_k \, \hat{\mathfrak{M}} \, \widehat{\mathbf{\Pi}}_k = \widehat{\mathbf{\Pi}}_k,$$

where

$$\widehat{\mathbf{\Pi}}_k := \widehat{\Pi}_k \mathbf{I}, \quad \widehat{\Pi}_k := \lim_{x \to \infty} e^{-\varpi_{\mathrm{i}}(\hat{p})x}$$

projects $\psi = \psi_{\rm osc} + \psi_{\rm ev}$ to $\psi_{\rm osc}$. $\psi_{\rm osc}$ is a combination of Fourier modes $\mathbf{p}$ such that $\|\mathbf{p}\| \leq k$ while $\psi_{\rm ev}$ is a combination of Fourier modes $\mathbf{p}$ such that $\|\mathbf{p}\| > k$.

Theorem

Let α be a positive real number, $\vec{e}$ be a unit vector lying in the $\mathbf{y}$ plane, and $v : \mathbb{R}^{D+1} \to \mathbb{C}$ be a short-range potential such that $\tilde{v}(x, \vec{\mathfrak{K}}) = 0$ for $\vec{\mathfrak{K}} \cdot \vec{e} \leq 2\alpha$. Then v is omnidirectionally invisible for every wavenumber k that does not exceed α.

Hint: For such potentials

$$\widehat{\mathscr{V}}(x)\,\widehat{\Pi}_k = \mathbf{0}.$$

This implies that for all $n \in \mathbb{Z}^+$ and $x_1, x_2, \cdots, x_n \in \mathbb{R}$,

$$\widehat{\mathbf{\Pi}}_k \widehat{\boldsymbol{\mathcal{H}}}(x_n)\widehat{\boldsymbol{\mathcal{H}}}(x_{n-1}) \cdots \widehat{\boldsymbol{\mathcal{H}}}(x_1)\widehat{\mathbf{\Pi}}_k = \widehat{\mathbf{0}}.$$

Theorem

Let $\xi \in [0, 2\pi)$, $\alpha, \beta \in \mathbb{R}^+$, $k \in (0, \alpha]$, and $v : \mathbb{R}^3 \to \mathbb{C}$ be a short-range potential such that for all $z \in \mathbb{R}$, $\tilde{\tilde{v}}(\vec{\mathfrak{K}}, z) = 0$ for $\mathfrak{K}_1 \leq \beta$. Then, $\widehat{\breve{\mathbf{M}}} = \widehat{\mathbf{I}}$ for $\beta \geq 2\alpha$, and

$$\widehat{\breve{\mathbf{M}}} = \widehat{\mathbf{I}} + \sum_{n=1}^{\lceil 2\alpha/\beta - 1 \rceil} (-i)^n \int_{z_0}^{z} dz_n \int_{z_0}^{z_n} dz_{n-1} \cdots \int_{z_0}^{z_2} dx_1 \Big[\widehat{\mathbf{\Pi}}_k \widehat{\breve{\boldsymbol{\mathcal{H}}}}(z_n) \widehat{\breve{\boldsymbol{\mathcal{H}}}}(z_{n-1}) \cdots \widehat{\breve{\boldsymbol{\mathcal{H}}}}(z_1) \widehat{\mathbf{\Pi}}_k \Big],$$

for $0 < \beta < 2\alpha$.

Corollary: Let α be a positive real number, $\vec{e}$ be a unit vector lying in the **y** plane, and v be a short-range potential such that $\tilde{v}(x, \vec{\mathfrak{K}}) = 0$ for $\vec{\mathfrak{K}} \cdot \vec{e} \leq \alpha$. Then the first Born approximation gives the exact expression for the scattering amplitude of v for wavenumbers $k \leq \alpha$,

Implicit regularization of delta-function potential in 2D

Suppose that the potential is given by

$$v(\boldsymbol{\rho}) = \mathfrak{z}\,\delta^2(\boldsymbol{\rho} - \boldsymbol{\rho}_0), \qquad \boldsymbol{\rho} := (x, y),$$

with $\mathfrak{z} \in \mathbb{C}$ and $\boldsymbol{\rho}_0 \in \mathbb{R}^2$.

1. The coupling constant $\mathfrak{z}$ is dimensionless.
2. The Schrodinger equation is invariant under $\boldsymbol{\rho} \to \lambda\boldsymbol{\rho}$, $\lambda > 0$.
3. The scattering amplitude is logarithmically UV divergent.

Transfer Matrix

Transfer matrix gives the correct scattering amplitude without consulting a regularization scheme.
Consider a left incident wave. We should solve the equation

$$\begin{bmatrix} A_+(p) \\ 0 \end{bmatrix} = \left(\widehat{\mathbf{I}} + \widehat{\mathbf{m}}\right) \begin{bmatrix} 2\pi\delta(p - p_0) \\ B_-(p) \end{bmatrix}$$

where

$$\widehat{\mathbf{m}} := -\frac{i\mathfrak{z}}{2\varpi(p)} e^{-i\varpi(p)a\sigma_3} \boldsymbol{\mathcal{K}} \widehat{\mathbf{\Pi}}_k \delta(i\partial_p - b) \widehat{\mathbf{\Pi}}_k e^{i\varpi(p)a\sigma_3}$$

and we have assumed $\boldsymbol{\rho}_0 = (a, b)$.

$$\widehat{\mathbf{m}}\begin{pmatrix} 2\pi\delta(p-p_0) \\ B_-(p) \end{pmatrix} = -\frac{i\mathfrak{z}\, c}{2\varpi(p)} e^{-ipb} e^{-i\varpi(p)a\sigma_3} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$c := e^{i\mathbf{p}_0\cdot\boldsymbol{\rho}_0} + \mathcal{F}^{-1}_{p,b}\{e^{-i\varpi(p)a} B_-(p)\} \tag{2}$$

This gives

$$B_-(p) = -\frac{i\mathfrak{z}\, c}{2\varpi(p)} e^{-ipb} e^{i\varpi(p)a}, \qquad p \in (-k, k) \tag{3}$$

Using (3) in (2) we can compute c. Using it in (3) we obtain

$$B_-(p) = -\frac{i}{2\varpi(p)} \frac{\mathfrak{z}}{1+\frac{i\mathfrak{z}}{4}} e^{i(\mathbf{p}_0-\mathbf{p})\cdot\boldsymbol{\rho}_0}$$

We note that for $\rho \to \infty$ and $\theta \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right)$

$$\begin{aligned}\psi_{\text{scat}}(\rho) &= \frac{1}{2\pi}\int_{-k}^{k} dp B_-(p) e^{ipy} e^{-i\varpi(p)x} \\ &\to -\frac{i\mathfrak{z}}{4+i\mathfrak{z}} e^{-i\pi/4}\sqrt{\frac{2}{\pi k\rho}} e^{ik\rho}\end{aligned}$$

Lippmann-Schwinger equation

$$\psi_{\text{scat}}(\boldsymbol{\rho}) = -\frac{i\mathfrak{z}(k)}{4 + i\mathfrak{z}} \sqrt{\frac{2}{\pi k \rho}} e^{-i\pi/4} e^{ik\rho}$$

where

$$\frac{1}{\mathfrak{z}(k)} = \frac{1}{\mathfrak{z}(k_{\text{ref}})} - \frac{1}{2\pi} \ln\left(\frac{k}{k_{\text{ref}}}\right)$$