Integral Equations in Quantum Mechanics II

I Bound States, II Scattering*

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Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

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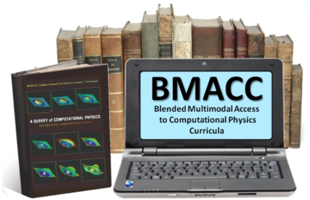
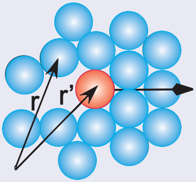
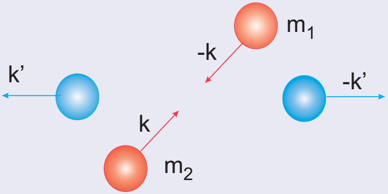
Course: **Computational Physics II**



Problem: Nonlocal Potential Scattering

Integro-Differential Equation





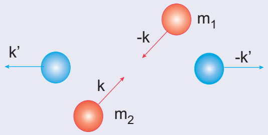
- **Problem:** Scattering from nonlocal potential

$$-\frac{1}{2m}\frac{d^2\psi(r)}{dr^2} + \int dr' \; V(r,r')\psi(r') = E\psi(r) \qquad (1)$$

- Avoid Integro-Differential Equation

Theory: Lippmann–Schwinger Equation

Integral Form Schrödinger Equation



- Better solve scattering amplitudes = observable ($\neq \psi$)
- $\mathcal{P}$ = Cauchy principal-value prescription; $l = 0$, $\hbar = 1$

$$R(k', k) = V(k', k) + \frac{2}{\pi}\mathcal{P}\int_0^\infty dp\, \frac{p^2 V(k', p) R(p, k)}{(k_0^2 - p^2)/2\mu} \tag{1}$$

$$E = \frac{k_0^2}{2\mu}, \quad \mu = \frac{m_1 m_2}{m_1 + m_2} \tag{2}$$

Math: Computing Singular Integrals

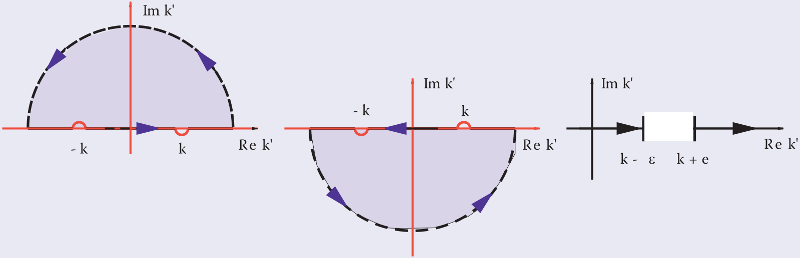
How Handle Singularity?

- Singular integral $\mathcal{G}$ has singular integrand $g(k)$:

$$\mathcal{G} = \int_a^b g(k)\, dk \neq \infty \tag{1}$$

- Computational danger near singularity

What to Do at Singularity?



- Give energy k_0 small imaginary part $\pm i\epsilon$
- Cauchy principal-value $\mathcal{P}$ = pinch*

$$\mathcal{P}\int_{-\infty}^{+\infty} f(k)\, dk \;=\; \lim_{\epsilon\rightarrow 0}\left[\int_{-\infty}^{k_0-\epsilon} f(k)\, dk + \int_{k_0+\epsilon}^{+\infty} f(k)\, dk\right] \tag{1}$$

Numerical Principal Values

Subtract Zero Integral (Hilbert Transform)

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{dk}{k-k_0} = \mathcal{P}\int_0^{+\infty} \frac{dk}{k^2-k_0^2} = 0 \tag{1}$$

$$\mathcal{P}\int_0^{+\infty} \frac{f(k)\,dk}{k^2-k_0^2} = \int_0^{+\infty} \frac{[f(k)-f(k_0)]\,dk}{k^2-k_0^2} \tag{2}$$

- NB No RHS $\mathcal{P}$, no $k = k_0$ singularity

Method: Integral- to Linear- to Matrix-Equations

Rewrite Principal-Value as Definite Integral

$$R(k',k) = V(k',k) + \frac{2}{\pi}\int_0^\infty dp\, \frac{p^2 V(k',p)R(p,k) - k_0^2 V(k',k_0)R(k_0,k)}{(k_0^2 - p^2)/2\mu} \quad (1)$$

- Convert to linear equations; approximate integral:

$$R(k,k_0) \simeq V(k,k_0) + \frac{2}{\pi}\sum_{j=1}^{N} \frac{k_j^2 V(k,k_j)R(k_j,k_0)w_j}{(k_0^2 - k_j^2)/2\mu} - \frac{2}{\pi}k_0^2 V(k,k_0)R(k_0,k_0)\sum_{m=1}^{N}\frac{w_m}{(k_0^2 - k_m^2)/2\mu} \quad (2)$$

- $(N+1)$ unknown $R(k_j,k_0)$, $j = 0, N$

Method: Integral- to Linear- to Matrix-Equations

Evaluate for $k = N$ Gauss Points k + Experimental k_0

$$k = k_i = \begin{cases} k_j, & j = 1, N \quad \text{(quadrature points)}, \\ k_0, & i = 0 \quad \text{(experimental point)} \end{cases} \tag{1}$$

$$R_i = V_i + \frac{2}{\pi} \sum_{j=1}^{N} \frac{k_j^2 V_{ij} R_j w_j}{(k_0^2 - k_j^2)/2\mu} - \frac{2}{\pi} k_0^2 V_{i0} R_0 \sum_{m=1}^{N} \frac{w_m}{(k_0^2 - k_m^2)/2\mu} \tag{2}$$

- Express as matrix equations:

$$D_i = \begin{cases} +\frac{2}{\pi} \frac{w_i k_i^2}{(k_0^2 - k_i^2)/2\mu}, & \text{for } i = 1, N, \\ -\frac{2}{\pi} \sum_{j=1}^{N} \frac{w_j k_0^2}{(k_0^2 - k_j^2)/2\mu}, & \text{for } i = 0 \end{cases} \tag{3}$$

$$R = V + DVR \quad \Rightarrow \quad R = (1 - DV)^{-1} V \tag{4}$$

Solution via Matrix Inversion, Gaussian Elimination

CODE

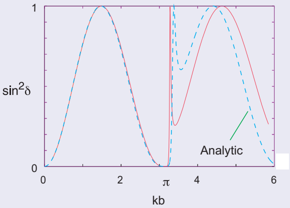
$$R = V + DVR \tag{1}$$

$$R = (1 - DV)^{-1} V \tag{2}$$

- Matrix inversion = direct, not fastest
- Matrix inversion = standard in mathematical libraries
- Useful if need $[1 - DV]^{-1}$
- Else Gaussian elimination

Implementation: Delta-Shell Potential

$\sin^2 \delta_0 \propto \; l = 0$ Cross Section



$$V(k', k) = \frac{-|\lambda| \sin(k'b) \sin(kb)}{2\mu k' k} \quad (1)$$

- Check analytic phase shift:

$$\tan \delta_0 = \frac{\lambda b \sin^2(kb)}{kb - \lambda b \sin(kb) \cos(kb)} \quad (2)$$

$$R(k_0, k_0) = -\frac{\tan \delta}{2\mu k_0} \quad (3)$$

- Estimate precision by increasing N grid points ($N = 26$)