Integral Equations in Quantum Mechanics I

I Bound States, II Scattering*

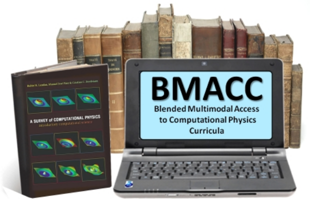
Rubin H Landau

Sally Haerer, Producer-Director

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

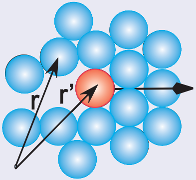
with Support from the National Science Foundation

Course: **Computational Physics II**



Problem: Bound States in Momentum Space

Integro-Differential Equation



- N–body interaction reduces to nonlocal $V_{eff}(r)$:

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

- Integro-differential equation
- **Problem:** Solve for $l = 0$ bound-state E_i & ψ_i

Theory: Momentum-Space Schrödinger Equation

Integral Schrödinger Equation Equally Valid

- Transform Schrödinger Equation to momentum space
- Replace integro-differential by integral equation:

$$\frac{k^2}{2\mu}\psi(k) + \frac{2}{\pi}\int_0^\infty dp p^2 V(k,p)\psi(p) = E\psi(k) \tag{1}$$

- $V(k,p)$= p-space representation (TF) of V:

$$V(k,p) = \frac{1}{kp}\int_0^\infty dr\, dr'\ \sin(kr)\, V(r,r')\ \sin(pr') \tag{2}$$

- $\psi(k)$ = p-space representation (TF) of ψ:

$$\psi(k) = \int_0^\infty dr\, kr\, \psi(r) \sin(kr) \tag{3}$$

- Will transform into matrix equation (see matrix Chapter)

Algorithm: Integral Equations → Linear Equations

Solve on p-Space Grid

$k_1 \quad k_2 \quad k_3 \quad \bullet \quad \bullet \quad \bullet \quad k_N$

- Integral $\simeq$ weighted sum (see Integration chapter)

$$\int_0^\infty dp p^2 V(k,p)\psi(p) \simeq \sum_{j=1}^{N} w_j k_j^2 V(k,k_j)\psi(k_j) \tag{1}$$

- Integral equation → algebraic equation

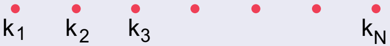
$$\frac{k^2}{2\mu}\psi(k) + \frac{2}{\pi}\sum_{j=1}^{N} w_j k_j^2 V(k,k_j)\psi(k_j) = E \tag{2}$$

- N unknowns $\psi(k_j)$
- 1 unknown E
- Unknown function $\psi(k)$

- Solve on grid, $k = k_i$
- $\rightarrow$ N couple equations
- $(N+1)$ unknowns:

Algorithm: Integral Equations → Linear Equations

Solve on p-Space Grid



$$\frac{k_i^2}{2\mu}\psi(k_i) + \frac{2}{\pi}\sum_{j=1}^{N} w_j k_j^2 \; V(k_i, k_j)\psi(k_j) = E\psi(k_i), \quad i = 1, N \tag{1}$$

- e.g. $N = 2 \;\Rightarrow$ 2 coupled linear equations

$$\frac{k_1^2}{2\mu}\psi(k_1) + \frac{2}{\pi} w_1 k_1^2 \; V(k_1, k_1)\psi(k_1) + w_2 k_2^2 \; V(k_1, k_2)\psi(k_2) \; = E\psi(k_1) \tag{2}$$

$$\frac{k_2^2}{2\mu}\psi(k_2) + \frac{2}{\pi} w_1 k_1^2 \; V(k_2, k_1)\psi(k_1) + w_2 k_2^2 \; V(k_2, k_2)\psi(k_2) \; = E\psi(k_2) \tag{3}$$

Algorithm: Integral Equations → Linear Equations

Solve on p-Space Grid k_1 k_2 k_3 k_N

$$\frac{k_i^2}{2\mu}\psi(k_i) + \frac{2}{\pi}\sum_{j=1}^{N} w_j k_j^2 \; V(k_i, k_j)\psi(k_j) = E\psi(k_i), \quad i = 1, N \tag{1}$$

- Matrix Schrödinger equation $[H][\psi] = E[\psi]$
- $\psi(k)$ = $N \times 1$ vector

$$\begin{pmatrix} \frac{k_1^2}{2\mu} + \frac{2}{\pi}V(k_1,k_1)k_1^2 w_1 & \frac{2}{\pi}V(k_1,k_2)k_2^2 w_2 & \cdots & \frac{2}{\pi}V(k_1,k_N)k_N^2 w_N \\ \cdots & \cdots & \cdots & \frac{k_N^2}{2\mu} + \frac{2}{\pi}V(k_N,k_N)k_N^2 w_N \end{pmatrix} \times \begin{pmatrix} \psi(k_1) \\ \psi(k_2) \\ \ddots \\ \psi(k_N) \end{pmatrix}$$

$$= E \begin{pmatrix} \psi(k_1) \\ \psi(k_2) \\ \ddots \\ \psi(k_N) \end{pmatrix} \tag{2}$$

Eigenvalue Problem

Search for Solution; N equations for $(N+1)$ unknowns?

- Solution only sometimes, certain E (eigenvalues)
- Try to solve, multiply both sides by $[H-EI]$ inverse:

$$[H][\psi] = E[\psi] \tag{1}$$

$$[H-EI][\psi] = [0] \tag{2}$$

$$\Rightarrow [\psi] = [H-EI]^{-1}[0] \tag{3}$$

- $\Rightarrow$ if inverse $\exists$, then only trivial solution $\psi \equiv 0$
- For nontrivial solution inverse can't $\exists$

$$\det[H-EI] = 0 \qquad \text{(bound-state condition)} \tag{4}$$

- Requisite additional equation for $N+1$ unknowns
- Solve for just eigenvalues, or full e.v. problem

Model: Delta-Shell Potential (Sort of Analytic Solution)

2 Particles Interact When b Apart

$$V(r) = \frac{\lambda}{2\mu}\delta(r-b) \tag{1}$$

$$V(k',k) = \frac{1}{k'k}\int_0^\infty \sin(k'r')\frac{\lambda}{2\mu}\delta(r-b)\sin(kr)\,dr \tag{2}$$

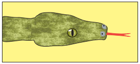
$$= \frac{\lambda}{2\mu}\frac{\sin(k'b)\sin(kb)}{k'k} \qquad \text{(too slow decay)} \tag{3}$$

- 1 Bound state $E = -\kappa^2/2\mu$, if

$$e^{-2\kappa b} - 1 = \frac{2\kappa}{\lambda} \tag{4}$$

- Only if strong & attractive ($\lambda < 0$)
- **Exercise:** Solve transcendental equation ($b = 10$, $\lambda = ?$)

Bound–State Integral–Equation Code



CODE

Sample Code Surveys all Parameters

- Gauss quadrature for pts & wts
- Two possible libe calls
- 1. Search on E, $\det[H - EI] = 0$
- 2. Use eigenproblem solver*
- Both iterative solutions

Your Implementation

Modify or Write Eigenvalues, Eigenproblem

1. $2\mu = 1$, $b = 10$, $N > 16$
2. Set up $[V(i,j)]$ and $[H(i,j])$ for $N \geq 16$
3. Observe monotonic relation $E(\lambda)$
4. True bound state stable with N, others = artifacts
5. Extract best value for E & estimate precision
6. Comparing RHS, LHS $[H][\psi] = E[\psi]$

Exploration: Momentum Space Wave Function*

Bound in p Space?

1. Determine $\psi(k)$ (analytic $\psi(p) \propto [p^2 - 2mE]^{-1}$)
2. Is this reasonable, normalizable?
3. Determine $\psi(r)$ via transform

$$\psi(r) = \int_0^\infty dk \psi(k) \frac{\sin(kr)}{kr} k^2 \tag{1}$$

4. Is this reasonable $\psi(r)$?
5. Compare to analytic $\psi(r)$,

$$\psi_0(r) \propto \begin{cases} e^{-\kappa r} - e^{\kappa r}, & \text{for } r < b, \\ e^{-\kappa r}, & \text{for } r > b \end{cases} \tag{2}$$