Schrödinger equation and single particle propagator.

How to generate possible discrete states of H from the propagator equation for G

We separate the spectrum of H in two parts: a discrete part and a continuous part

Discrete

$$H|n\rangle = \varepsilon_n |n\rangle$$
$$\varepsilon_n < 0$$

Continuum

$$H|\mu\rangle = \varepsilon_\mu |\mu\rangle$$
$$\varepsilon_\mu > 0$$

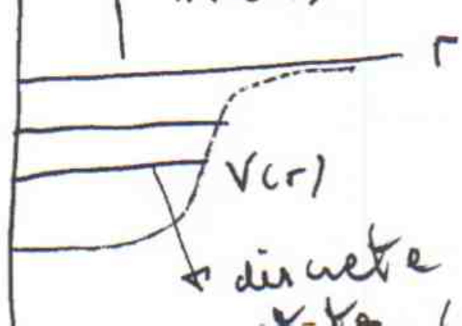
Completeness relation:

$$1 = \sum_n |n\rangle\langle n| + \int d\mu\, |\mu\rangle\langle\mu|$$

Therefore the propagator in any basis

$$\boxed{G(\alpha,\beta;E) = \sum_n \frac{\langle\alpha|n\rangle\langle n|\beta\rangle}{E-\varepsilon_n+i\eta} + \int d\mu\, \frac{\langle\alpha|\mu\rangle\langle\mu|\beta\rangle}{E-\varepsilon_\mu+i\eta}}$$

$$H = \underset{\substack{\downarrow\\ \text{kinetic}\\ \text{energy}}}{T} + \underset{\substack{\downarrow\\ \text{energy independent}\\ \text{potential } V(r)}}{V}$$



Let's try to recover the Schrödinger equation for bound states from the equation for the propagator. We will make use of the spectral representation and will work in the momentum basis!

Let's calculate the following limit:

$$\lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n)\left\{ G = G^{(0)} + G^{(0)} V G \right\}$$

$\mathcal{E}_n$ is the energy of a bound state.

Let's look at the different pieces of the limit:

(1) $$\lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n) G = \lim_{E\to\mathcal{E}_n} \left\{ \sum_m' \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E-\mathcal{E}_m+i\eta} + \int d\mu \ldots \right\}$$

$$= \langle\alpha|n\rangle\langle n|\beta\rangle \Rightarrow \langle\vec{p}|n\rangle\langle n|\vec{p}\,'\rangle$$ in the momentum basis.

(2) $$\lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n) G^{(0)} = \lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n)\langle\alpha|\frac{1}{E-T+i\eta}|\beta\rangle$$

$$\Rightarrow \lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n)\frac{\delta(\vec{p}-\vec{p}\,')}{E-\frac{p^2}{2m}+i\eta} \to 0$$

(3) $$\lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n) G^{(0)} V G = \lim_{E\to\mathcal{E}_n} (E-\mathcal{E}_n)$$

$$\sum_{\gamma\delta}' \langle\alpha|\frac{1}{E-T+i\eta}|\gamma\rangle\langle\gamma|V|\delta\rangle \left\{ \sum_m' \frac{\langle\delta|m\rangle\langle m|\beta\rangle}{E-\mathcal{E}_m+i\eta} + \int d\mu \ldots \right\}$$

$$= \sum_{\gamma\delta}' \langle\alpha|\frac{1}{E-T}|\gamma\rangle\langle\gamma|V|\delta\rangle\langle\delta|n\rangle\langle n|\beta\rangle \Rightarrow$$ momentum

$$\Rightarrow \sum_{\gamma\delta} \langle \alpha | \frac{1}{\varepsilon_n - T} | \gamma \rangle \langle \gamma | V | \delta \rangle \langle \delta | n \rangle \langle n | \beta \rangle \Rightarrow$$

$$\langle \vec{k}_1 | \frac{1}{\varepsilon_n - T} \int d^3k \, |\bar{k}\rangle \langle \bar{k} | V | \int d^3k' \, |\bar{k}'\rangle \langle \bar{k}' | n \rangle \langle n | \vec{k}_2 \rangle$$

$$\Rightarrow \int d^3k \, d^3k' \, \frac{\delta(\bar{k}_1 - \bar{k})}{\varepsilon_n - \frac{\hbar^2 k_1^2}{2m}} \langle \bar{k} | V | \bar{k}' \rangle \langle \bar{k}' | n \rangle \langle n | \bar{k}_2 \rangle$$

$$\Rightarrow \int d^3k' \, \frac{1}{\varepsilon_n - \frac{\hbar^2 k_1^2}{2m}} \langle \bar{k}_1 | V | \bar{k}' \rangle \langle \bar{k}' | n \rangle \langle n | \bar{k}_2 \rangle$$

Collecting the terms from the left hand side:

$$\underbrace{\langle \vec{k}_1 | n \rangle}_{\text{wave function in momentum space } \phi_n(k_1)} \cancel{\langle n | \vec{k}_2 \rangle} = \frac{1}{\varepsilon_n - \frac{\hbar^2 k_1^2}{2m}} \cancel{\langle n | \bar{k}_2 \rangle} \int d^3k' \langle \bar{k}_1 | V | \bar{k}' \rangle \langle \bar{k}' | n \rangle$$

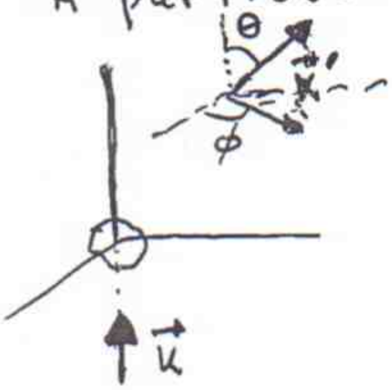
$$\left[- \frac{\hbar^2 k_1^2}{2m} + \varepsilon_n \right] \phi_n(k_1) = \int d^3k' \langle \bar{k}_1 | V | \bar{k}' \rangle \, \phi_n(\bar{k}')$$

$$\boxed{\frac{\hbar^2 k_1^2}{2m} \phi_n(\bar{k}_1) + \int d^3k' \langle k_1 | V | k' \rangle \phi_n(\bar{k}') = \varepsilon_n \phi_n(\bar{k}_1)}$$

Schrödinger equation in momentum space!

Scattering

A particle scatters with a potential.



$$H = H_0 + V(r) \qquad H_0 = \frac{p^2}{2m}$$

$V(r)$ $\downarrow$ localized potential

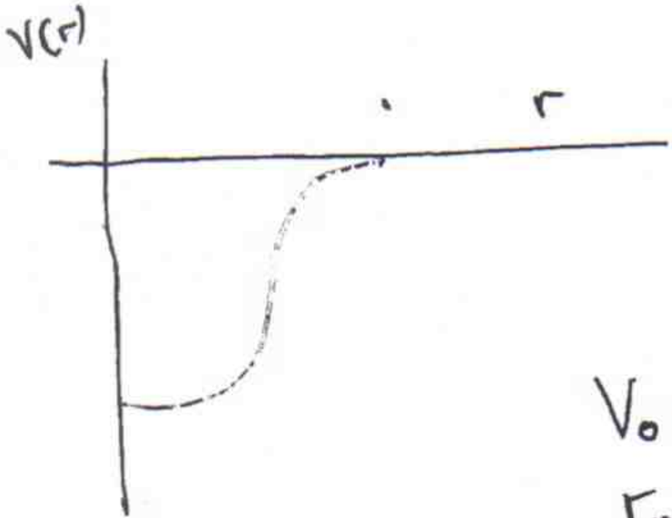
→ Elastic scattering $|\vec{k}| = |\vec{k}'|$.
Only can change the direction of the incident momentum!

→ Usually one considers that $\vec{k}$ propagate along the z-axis towards a target located at the origin. Detection takes place in a direction pointing away from the origin, specified by the angles θ, ϕ.

→ Differential cross section ⟺ scattering amplitude ⟺ matrix element of the T-matrix

$$\boxed{\begin{aligned}
&\frac{d\sigma}{d\Omega} = \left| f_E(\theta,\phi) \right|^2 \\
&f_E(\theta,\phi) = -\frac{4m\pi^2}{\hbar^2} \langle \vec{k}' | T\Big(E = \underbrace{\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (k')^2}{2m}}_{}\Big) | \vec{k} \rangle \quad \text{elastic!} \\
&\langle \vec{r} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{r}}
\end{aligned}}$$

Scattering of a particle with an external potential



$$V(r) = \frac{V_0}{1 + e^{\frac{r - r_0}{\alpha}}}$$

$V_0 = -50.$ MeV

$r_0 = 3.1$ fm

$\alpha = 0.4$ fm

$$\boxed{T = V + V \frac{1}{E - H_0 + i\eta} T}$$

$$H_0 |\vec{q}\rangle = \frac{\hbar^2 q^2}{2m} \qquad \frac{1}{E - H_0 + i\eta} = \int d^3q \, \frac{|\vec{q}\rangle\langle\vec{q}|}{E - \frac{\hbar^2 q^2}{2m} + i\omega}$$

$$I = \int d^3r \, |\vec{r}\rangle\langle\vec{r}| = \int d^3k \, |\vec{k}\rangle\langle\vec{k}|$$

$$\langle\vec{r}|\vec{k}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{r}}$$

The elastic collision process is fully defined by a matrix element of the T-matrix.

$$\boxed{\langle\vec{k}|T(E)|\vec{k}'\rangle = \langle\vec{k}|V|\vec{k}'\rangle + \int d^3q\, \langle\vec{k}|V|\vec{q}\rangle \frac{1}{E-\frac{\hbar^2 q^2}{2m}+i\eta}\langle\vec{q}|T|\vec{k}'\rangle}$$

Convenient to perform a partial wave decomposition!

$$\langle\vec{k}|V|\vec{k}'\rangle = \frac{1}{(2\pi)^3}\int d^3r\, e^{-i\vec{k}\vec{r}}\, V(r)\, e^{i\vec{k}'\vec{r}}$$

$$= \sum_{lm} V_l(k,k')\, Y^*_{lm}(\hat{k})\, Y_{lm}(\hat{k}')$$

$$V_l(k,k') = \frac{2}{\pi}\int dr\, r^2\, j_l(kr)\, V(r)\, j_l(k'r)$$

we will explicitly work with $l=0$

$$V_0(k,k') = \frac{2}{\pi k k'}\int dr\, \sin(kr)\, \sin(k'r)\, V(r)$$

How is written the equation in partial waves?

$$\boxed{T_l(E,k,k') = V_l(k,k') + \int_0^\infty dq\, q^2\, \frac{V_l(k,q)\, T_l(q,k')}{E-\frac{\hbar^2 q^2}{2m}+i\eta}}$$

For $E>0 \Rightarrow T$ will be complex

$$\frac{1}{E-H_0+i\eta} = \mathcal{P}\frac{1}{E-H_0} - i\pi\delta(E-H_0)$$

If we have two integral equations that differ only in the propagator

$$T = V + V\, P^{T}_{prop}\, T \qquad R = V + V\, P^{R}_{prop}\, R$$

$$P^{T}_{prop} = \frac{1}{E-H_0+i\eta} \qquad P^{R}_{prop} = \mathcal{P}\frac{1}{E-H_0}$$

one can derive an integral equation relating T and R.

$$T = R + R\left\{P^{T}_{prop} - P^{R}_{prop}\right\} T$$

$$P^{T}_{prop} - P^{R}_{prop} = -i\pi\delta(E-H_0)$$

$$R_\ell(E,k,k') = V_\ell(k,k') + \mathcal{P}\int dq\, q^2\, \frac{V_\ell(k,q)\, R_\ell(q,k')}{E-\frac{\hbar^2 q^2}{2m}}$$

$$T_\ell(E,k,k') = R_\ell(E,k,k') - i\pi\int dq\, q^2\, R_\ell(k,q)\, \delta\!\left(E-\frac{\hbar^2 q^2}{2m}\right) T_\ell(E,q,$$

Assuming that we have R_ℓ, how to solve the second equation?

Let's assume $E = \frac{\hbar^2 k_p^2}{2m} \rightarrow$ at $k = k_p$

the equation for R_ℓ will have a pole.

$$\delta(f(x)) = \left|\frac{df(x)}{dx}\right|^{-1}_{x=x_0} \delta(x - x_0) \qquad f(x_0) = 0$$

$$\left.\frac{\partial E(q)}{\partial q}\right|_{q=k_p} = \frac{\hbar^2 k_p}{m} \Rightarrow \delta(E - E(k_p)) = \frac{m}{\hbar^2 k_p}\delta(q - k_p)$$

$$T_\ell\left(E = \frac{\hbar^2 k_p^2}{2m}, k, k'\right) = R_\ell(E, k, k') - i\pi \int_0^\infty dq\, q^2\, \delta(q - k_p)\, R_\ell(E, k, q)\frac{m}{\hbar^2 k_p} T_\ell(E, q, k')$$

$\Rightarrow$

$$T_\ell(E, k, k') = R_\ell(E, k, k') - i\pi k_p^2 \cdot \frac{m}{\hbar^2 k_p} R_\ell(E, k, k_p) T_\ell(E, k_p, k')$$

in particular, I should find first $T_\ell(E, k_p, k')$

$$T_\ell(E, k_p, k') = R_\ell(E, k_p, k') - i\pi k_p^2 \frac{m}{\hbar^2 k_p} R_\ell(E, k_p, k_p) T_\ell(E, k_p, k')$$

$\Downarrow$

$$T_\ell(E, k_p, k') = \frac{R_\ell(E, k_p, k')}{1 + i\pi k_p^2 \frac{m}{\hbar^2 k_p} R_\ell(E, k_p, k_p)}$$

therefore,

$$\boxed{T_\ell(E, k, k') = R_\ell(E, k, k') - i\pi k_p^2 \frac{m}{\hbar^2 k_p} R_\ell(E, k, k_p) \cdot \frac{R_\ell(E, k_p, k')}{1 + i\pi k_p^2 \frac{m}{\hbar^2 k_p} R_\ell(k_p, k_p)}}$$

$$T_\ell(E, k_p, k') = \frac{R_\ell(k_p, k')}{1 + \frac{i\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}} R_\ell(E, k_p, k_p)}$$

$$= \frac{R_\ell(k_p, k')\left[1 - \frac{i\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}} R_\ell(E, k_p, k_p)\right]}{1 + \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 R_\ell^2(E, k_p, k_p)}$$

now we can use this $T_\ell(E, k_p, k')$ in the general matrix element

$$T_\ell(E, k, k') = R_\ell(E, k, k') - \frac{i\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}} R_\ell(E, k, k_p)\left[\frac{R_\ell(k_p, k')\left[1 - \frac{i\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}} R_\ell\right]}{1 + \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 R_\ell^2(E, k_p, k_p)}\right]$$

$$T_\ell(E, k, k') = R_\ell(E, k, k') - \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 \frac{R_\ell(E, k, k_p)\, R_\ell(k_p, k')\, R_\ell(k_p, k_p)}{1 + \left(\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right)^2 R_\ell^2(E, k_p, k_p)}$$

$$- i\left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right] \frac{R_\ell(k, k_p)\, R_\ell(k_p, k')}{1 + \left(\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right)^2 R_\ell^2(k_p, k_p)}$$

For $E > 0$ $T_\ell(E, k, k')$ is a complex object

$$\mathrm{Re}\left\{T_\ell(E, k, k')\right\}_{E=\frac{\hbar^2 k_p^2}{2m}} = R_\ell(k, k') - \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 \frac{R_\ell(k, k_p)\, R_\ell(k_p, k')\, R_\ell(k_p, k_p)}{1 + \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 R_\ell^2(k_p, k_p)}$$

$$\mathrm{Im}\left\{T_\ell(E, k, k')\right\} = - \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right] \frac{R_\ell(k, k_p)\, R_\ell(k_p, k')}{1 + \left[\frac{\pi k_p^2}{\left|\frac{\partial E}{\partial q}\right|_{k_p}}\right]^2 R_\ell^2(k_p, k_p)}$$

How to calculate R_ℓ?

$$R_\ell(E, k, k') = V_\ell(k, k') + P \int dq\, q^2 \frac{V_\ell(k, q)\, R_\ell(q, k')}{E - \frac{\hbar^2 q^2}{2m}}$$

For a given $E>0$, for $E = \frac{\hbar^2 k_p^2}{2m}$ the integral has a pole. One can try a special mesh to avoid k_p. However, it is more efficient to substract a quantity that is zero and makes the integrand smooth.

We substract:

$$k_p^2\, V_\ell(k, k_p)\, R_\ell(k_p, k') \cdot \lim_{q \to k_p} \left\{ \frac{q^2 - k_p^2}{\frac{\hbar^2 k_p^2}{2m} - \frac{\hbar^2 q^2}{2m}} \right\}$$

$$P \int^\infty \frac{dq}{q^2 - k_p^2} \equiv 0$$

$$R_\ell(k,k') = V_\ell(k,k') + P\int_0^\infty dq\, q^2 \frac{V_\ell(k,q) R_\ell(q,k')}{E - \frac{\hbar^2 q^2}{2m}}$$

$$- B(k_p)\, V_\ell(k,k_p)\, R_\ell(k_p,k') \cdot P \int \frac{dq}{q^2 - k_p^2}$$

$$B(k_p) = k_p^2 \lim_{q\to k_p} \left\{ \frac{q^2 - k_p^2}{\frac{\hbar^2 k_p^2}{2m} - \frac{\hbar^2 q^2}{2m}} \right\}$$

$$\lim_{q\to k_p} \left\{ \frac{q^2 - k_p^2}{\frac{\hbar^2 k_p^2}{2m} - \frac{\hbar^2 q^2}{2m}} \right\} = -\frac{2m}{\hbar^2}$$

$$\boxed{B(k_p) = -\frac{k_p^2\, 2m}{\hbar^2}}$$

Discretization of the integral equation

$\Rightarrow$ Matrix inversion!

We choose a mesh and for each energy add k_p to the mesh $\Rightarrow$ that will be the $N+1$ point of the grid!

We now evaluate the discretize equation

at $k = k_i$, $i = 1, \ldots, N+1$; $k' = k_\ell$, $\ell = 1, \ldots, N+1$ $\Rightarrow$ a set of $(N+1)(N+1)$ equations, with $(N+1)(N+1)$ unknows $R_\ell(E, k_i, k_\ell)$ $i = 1 \ldots N+1$, $\ell = 1, \ldots, N+1$

$$\boxed{\begin{aligned} R_\ell(k_i, k_\ell, E) &= V_\ell(k_i, k_\ell) + \sum_{j=1}^{N} k_j^2 w_j \frac{V_\ell(k_i,k_j)\, R_\ell(k_j, k_\ell, E)}{E - \frac{\hbar^2 k_j^2}{2m}} \\ &- B(k_p) \left\{ \sum_{m=1}^{N} \frac{w_m}{k_m^2 - k_p^2} \right\} V_\ell(k_i, k_p)\, R_\ell(k_p, k_\ell, E) \\ & \qquad i = 1, \ldots, N+1 \\ & \qquad \ell = 1, \ldots, N+1 \end{aligned}}$$

defining

$$\begin{cases} W'_j = \dfrac{k_j^2 \, \omega_j}{E - \dfrac{\hbar^2 k_j^2}{2m}} & j = 1, \ldots, N \\[2ex] W'_{N+1} = - B(k_p) \displaystyle\sum_{m=1}^{N} \dfrac{\omega_m}{k_m^2 - k_p^2} & \end{cases}$$

$$\boxed{R_L(k_i, k_e, E) = V_L(k_i, k_e) + \sum_{j=1}^{N+1} V_L(k_i, k_j) \, W'_j \, R_L(k_j, k_e, E) \qquad \begin{array}{l} i = 1, \ldots, N+1 \\ j = 1, \ldots, N+1 \end{array}}$$

introducing the following matrix:

$$F_{ij} = \delta_{ij} - W'_j \, V_L(k_i, k_j)$$

$$\Downarrow$$

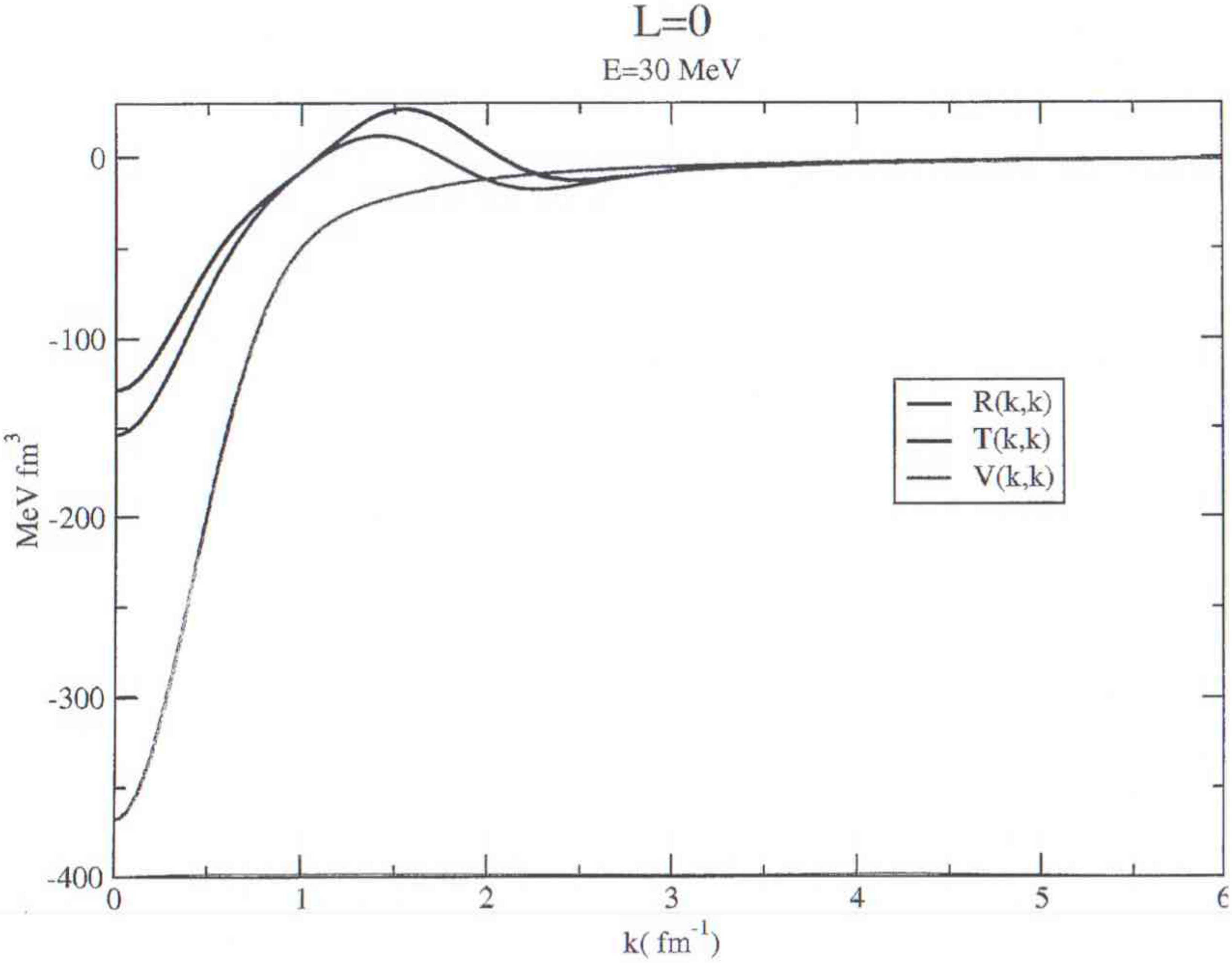
$$\boxed{\sum_{j=1}^{N+1} F_{ij} \, R_L(k_j, k_e, E) = V_L(k_i, k_e) \qquad \begin{array}{l} i = 1, \ldots, N+1 \\ j = 1, \ldots, N+1 \end{array}}$$

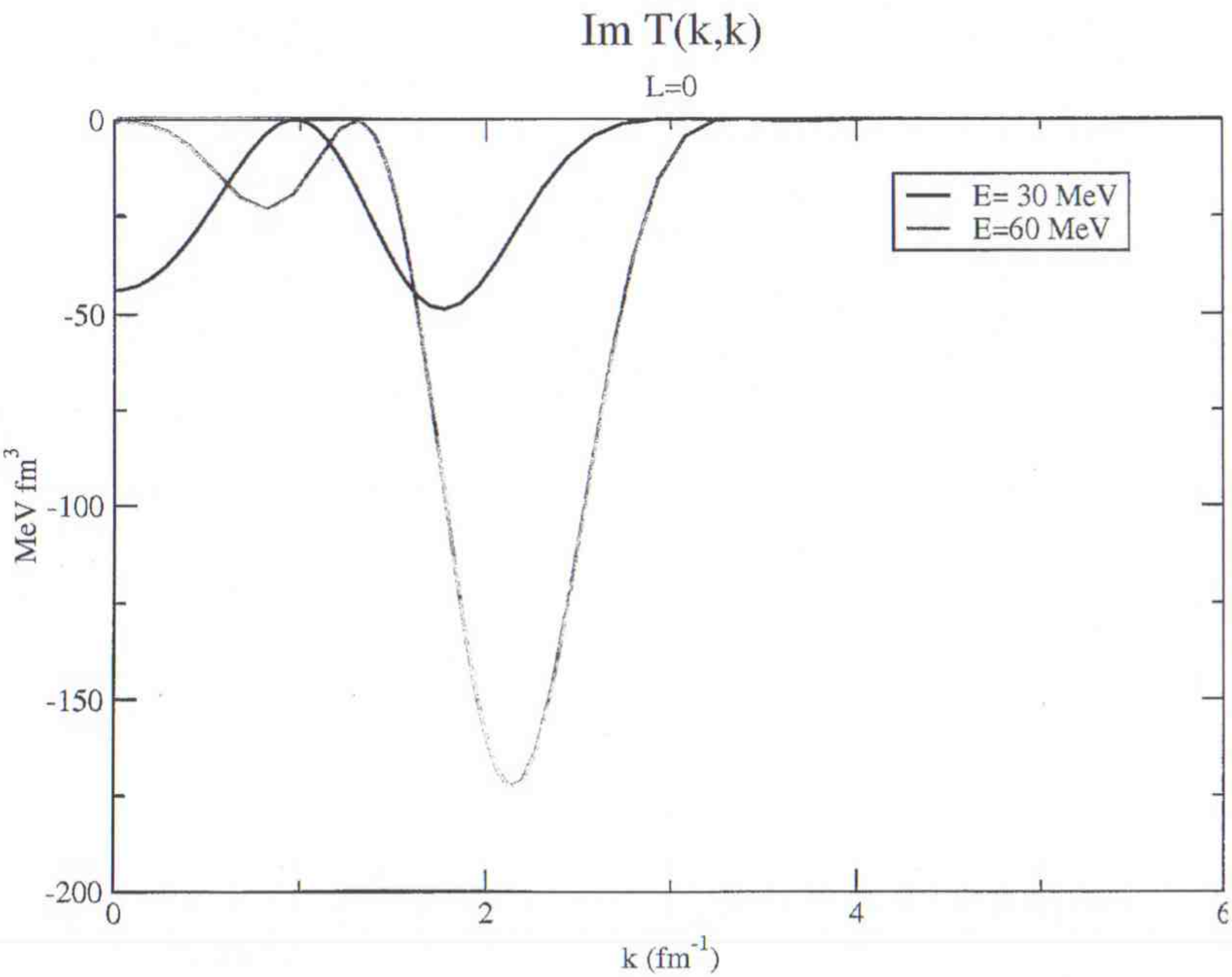
$$\Downarrow$$

which is solved numerically by <u>matrix inversion</u>!

$$R_L(k_i, k_L, E) = \sum_{j=1}^{N+1} (F)^{-1}_{ij} \, V_L(k_j, k_e)$$

$$\begin{bmatrix} 1-\dfrac{q_1^2 w_1 V_e(q_1,q_1)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_1^2}{2m}} & \cdots & -\dfrac{q_N^2 w_N V_e(q_1,q_N)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_N^2}{2m}} & -k_p^2 \dfrac{2m}{\hbar^2} \cdot V_e(q_1,k_p) \sum_{i=1}^{N} \dfrac{w_i}{q_i^2-k_p^2} \\ -\dfrac{q_1^2 w_1 V_e(q_2,q_1)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_1^2}{2m}} & 1-\dfrac{q_2^2 w_2 V_e(q_2,q_2)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_2^2}{2m}} \quad \cdots & & -k_p^2 \dfrac{2m}{\hbar^2} V_e(q_2,k_p) \sum_{i=1}^{N} \dfrac{w_i}{q_i^2-k_p^2} \\ \vdots & & & \vdots \\ -\dfrac{q_1^2 w_1 V_e(k_p,q_1)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_1^2}{2m}} & \cdots & -\dfrac{q_N^2 w_N V_e(k_p,q_N)}{\frac{\hbar^2 k_p^2}{2m}-\frac{\hbar^2 q_N^2}{2m}} & 1-k_p^2 \dfrac{2m}{\hbar^2} V_e(k_p,k_p) \sum_{i} \dfrac{w_i}{q_i^2-k_p^2} \end{bmatrix} \begin{bmatrix} R_e(q_1,q_e) \\ R_e(q_2,q_e) \\ \vdots \\ R_e(q_N,q_e) \\ R_e(k_p,q_e) \end{bmatrix} = \begin{bmatrix} V_e(q_1,q_e) \\ V_e(q_2,q_e) \\ \vdots \\ V_e(k_p,q_e) \end{bmatrix}$$


L=0
E=30 MeV
MeV fm^3
0
-100
-200
-300
-400
k(fm^{-1})
0
1
2
3
4
5
6
R(k,k)
T(k,k)
V(k,k)


Im T(k,k)
L=0
E= 30 MeV
E=60 MeV
MeV fm^3
k (fm^-1)
0
-50
-100
-150
-200
0
2
4
6