

A practical walk through formal scattering theory

**Connecting bound states, resonances, and scattering
states in exotic nuclei and beyond**

The Lippmann-Schwinger equation

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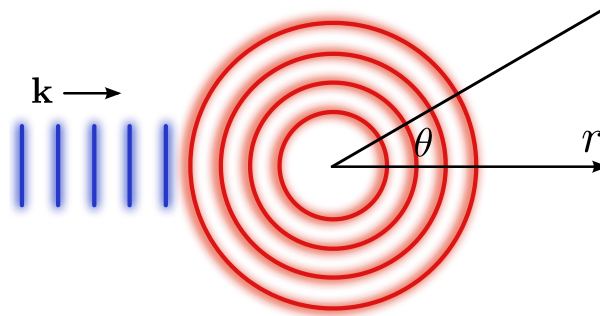


Theory
Alliance

Scattering setup

- we consider two particles with masses m_1 and m_2 at positions \mathbf{r}_1 and \mathbf{r}_2
- we assume that the interaction does not depend on absolute particle positions
- then we can **neglect the overall center-of-mass motion** and work only with the **relative coordinate** $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and **reduced mass** $\mu = m_1 m_2 / (m_1 + m_2)$
- for the two particles scattering off one another, we physically expect that the wavefunction describing their relative motion is given as a sum of an **incoming plane wave** and an **outgoing spherical scattered wave**:

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + f_k(\theta) \frac{e^{ikr}}{r} \quad (1)$$



- all physics information is contained in the **scattering amplitude** $f_k(\theta)$

Free Hamiltonian

- the **free Hamiltonian** H_0 is an important reference operator
 - differential operator ($\sim d^2/dr^2$) in configuration space
 - diagonal multiplicative operator in momentum space
- it has a **purely continuous spectrum** of plane-wave states:

$$H_0|\mathbf{k}\rangle = \frac{\mathbf{k}^2}{2\mu}|\mathbf{k}\rangle \quad (2)$$

- this is for a two-body system with **relative momentum \mathbf{k}** and **reduced mass μ**

Note

- the plane-wave states \mathbf{k} are not elements of the physical Hilbert space
 - $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$ is not a normalizable wavefunction ($\notin L^2(\mathbb{R}^3)$)
- strictly one should work with **wave packets** $|\phi\rangle \sim \int d^3p g(\mathbf{p})|\mathbf{p}\rangle$
- nevertheless it is **convenient and permissible** to work with plane-wave states because every element of the Hilbert space can be expanded in them (**Fourier transform!**)

Interaction potential

- we will consider generic potentials V written as **operators**
- we assume these potentials to be **time independent**, but they may in principle depend on energy, $V = V(E)$
- taking **matrix elements** gives a concrete representation, for example:

$$V(\mathbf{r}', \mathbf{r}) = \langle \mathbf{r}' | V | \mathbf{r} \rangle$$

- the most intuitive (and familiar) potentials are **local and spherically symmetric** in coordinate space: $V(\mathbf{r}', \mathbf{r}) = V(r)\delta^{(3)}(\mathbf{r} - \mathbf{r}')$, with $r = |\mathbf{r}|$

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- in the following, we will work in **momentum space**
- then $V(\mathbf{p}', \mathbf{p}) = \langle \mathbf{p}' | V | \mathbf{p} \rangle$ is related to $V(\mathbf{r}', \mathbf{r})$ by **Fourier transformation**
- we typically **project onto fixed partial waves**, denoted by l
- for local potentials, this leads to the following expression:

$$V_l(p', p) = 4\pi \int_0^\infty dr r^2 j_l(p'r) V(r) j_l(pr), \quad (3)$$

where $j_l(z)$ is the l -th **spherical Bessel function**

Partial-wave projected potentials

- numerically, it is better to use **Riccati-Bessel functions** $\hat{j}_l(z) = z j_l(z)$
- this explicitly reflects the cancellation of the singularity at $r = 0$

$$V_l(p', p) = \frac{4\pi}{p'p} \int_0^\infty dr \hat{j}_l(p'r) V(r) \hat{j}_l(pr) \quad (4)$$

Python implementation

```
# lib/potential.py

from scipy.integrate import quad

class LocalPotential(Potential):
    # [...]

    # Specific subclasses implement __call__(self, r)

    def get(self, ell, p, q):
        return 4.0 * np.pi / (q * p) * quad( \
            lambda r: riccati_j(ell, p * r) * self(r) * riccati_j(ell, q * r), \
            0.0, np.inf \
        )[0]
```

Plane-wave boundary condition

- consider the stationary Schrödinger equation: $H|\psi\rangle = E|\psi\rangle$ with $H = H_0 + V$
- this equation alone does not specify a boundary condition for solutions $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$
- a scattering state should be such that for $V \rightarrow 0$, $|\psi\rangle \rightarrow |\mathbf{k}\rangle$
- moreover, the state should be one that evolved from a free state in the infinite past

Interlude: time dependence

- the full Schrödinger equation is $i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle = (H_0 + V)|\psi(t)\rangle$
- Green's functions solve the time dependence:

$$G_0(t) = G_0^{(+)}(t) = \begin{cases} -ie^{-iH_0 t} & t > 0, \\ 0 & t \leq 0 \end{cases} \quad (5)$$

- ▶ this is the free **retarded** Green's function
 - ▶ advanced Green's functions vanish for $t \geq 0$
 - ▶ **full Green's functions** are defined analogously with $H_0 \rightarrow H$ in Eq. (5)
 - ▶ sometimes these operators are denoted by $U_0(t)$ and $U(t)$
- time dependence of waves is conventionally written $\sim e^{-iEt}$
 $\hookrightarrow e^{\pm ikr}$ represent in- and outgoing spherical waves, respectively
 - $G_0(z)$ is the Fourier transform $G_0(E)$ of $G_0(t)$, analytically continued into the whole complex energy plane

Interlude: adiabatic switching

- define a **free in state** that was equal to the exact interacting state in the infinite past:

$$|\psi_{\text{in}}(t)\rangle = \lim_{t' \rightarrow -\infty} iG_0^{(+)}(t - t')|\psi(t')\rangle \quad (6)$$

- this allows us to write down a formal solution using the full Green's function:

$$|\psi(t)\rangle = |\psi_{\text{in}}(t)\rangle + \lim_{\varepsilon \rightarrow 0^+} \int dt e^{-\varepsilon t'} G^{(+)}(t - t') V |\psi_{\text{in}}(t)\rangle \quad (7)$$

- if the states are monochromatic (fixed definite energy), the damping factor $e^{-\varepsilon t'}$ with $\varepsilon \rightarrow 0^+$ is required in Eq. (7)
- approximately this can be interpreted as multiplying the potential V with $e^{-\varepsilon t'}$, **adiabatically switching it off** in the infinite past
- when **wave packets** are used to represent proper physical scattering states, such damping factors are **not necessary**; their presence otherwise permits the convenience of working with simple plane-wave states

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- a scattering state should be such that for $V \rightarrow 0$, $|\psi\rangle \rightarrow |\mathbf{k}\rangle$
- moreover, the state should be one that evolved from a free state in the infinite past
- both conditions can be enforced with the ansatz

$$|\psi_{\mathbf{k}}^{(+)}\rangle = |\mathbf{k}\rangle + (E_{\mathbf{k}} - H_0 + i\varepsilon)^{-1} V |\psi_{\mathbf{k}}^{(+)}\rangle \quad (8)$$

with $E_{\mathbf{k}} = p^2/(2\mu)$

- this is the **Lippmann-Schwinger equation** for the scattering state $|\psi_{\mathbf{k}}^{(+)}\rangle$

Notes

- free Green's function $G_0(z) = (z - H_0)^{-1}$ appears in Eq. (8) with $z = E_{\mathbf{k}} + i\varepsilon$
- $\varepsilon \rightarrow 0$ is implied in all equations, this implements the adiabatic switching
- linear equation becomes an integral equation when projected onto a concrete representation

The Lippmann-Schwinger equation

- consider further Eq. (8) and apply V from the left:

$$V|\psi_{\mathbf{k}}^{(+)}\rangle = V|\mathbf{k}\rangle + VG_0(E_{\mathbf{k}} + i\varepsilon)V|\psi_{\mathbf{k}}^{(+)}\rangle \quad (9)$$

- define an operator T via $V|\psi_{\mathbf{k}}^{(+)}\rangle = T|\mathbf{k}\rangle$
 - for now, this merely **assumes** the existence of such an operator
 - it will be justified later
- using the definition of T , we can write:

$$T|\mathbf{k}\rangle = V|\mathbf{k}\rangle + VG_0(E_{\mathbf{k}} + i\varepsilon)T|\mathbf{k}\rangle \quad (10)$$

- this represents the **Lippmann-Schrödinger equation** for the operator T

Notes

- since \mathbf{k} is arbitrary in Eq. (10), we **postulate at the operator level**: $T = V + VG_0T$
- $T = T(E_{\mathbf{k}} + i\varepsilon)$ carries an implicit energy dependence via G_0
- alternative form: $T = V + TG_0V$ (seen to be equivalent by iteration)

The T-matrix

- in practice, we want an **explicit representation** of T
- we apply $\langle \mathbf{p} |$ from the left and define $T(E_{\mathbf{k}} + i\varepsilon; \mathbf{p}, \mathbf{k}) = \langle \mathbf{p} | T(E_{\mathbf{k}} + i\varepsilon) | \mathbf{k} \rangle$
- this is called the **T-matrix**, and it satisfies

$$\langle \mathbf{p} | T | \mathbf{k} \rangle = \langle \mathbf{p} | V | \mathbf{k} \rangle + \langle \mathbf{p} | V G_0(E_{\mathbf{k}} + i\varepsilon) T | \mathbf{k} \rangle \quad (11)$$

- Eq. (11) involves the **momentum-space potential** $V(\mathbf{p}, \mathbf{k}) = \langle \mathbf{p} | V | \mathbf{k} \rangle$
- to solve Eq. (11), we need to fully write out the second term on the right
 - insert complete sets of momentum states
 - note that Green's function is diagonal: $\langle \mathbf{q} | G_0(z) | \mathbf{q}' \rangle = G_0(z; \mathbf{q}) \delta^{(3)}(\mathbf{q} - \mathbf{q}')$

$$T(E_{\mathbf{k}} + i\varepsilon; \mathbf{p}, \mathbf{k}) = V(\mathbf{p}, \mathbf{k}) + \int \frac{d^3 q}{(2\pi)^3} V(\mathbf{p}, \mathbf{q}) G_0(E_{\mathbf{k}} + i\varepsilon; \mathbf{q}) T(E_{\mathbf{k}} + i\varepsilon; \mathbf{q}, \mathbf{k}) \quad (12)$$

- this **integral equation** can be solved numerically via **discretization**

Momentum discretization

Numerical quadrature

- a quadrature rule is a set of **mesh points** p_i together with **associated weights** w_i such that for a function $f(p)$ it holds that

$$\int_a^b f(p) \, dp \approx \sum_{i=1}^N w_i f(p_i) \quad (13)$$

- the interval boundaries may be among the p_i (closed rule) or not (open rule)
- increasing N improves the approximation in Eq. (13)

Mesh class

- a very common choice is **Gauss-Legendre quadrature**

```
from lib.mesh import *  
mesh = GaulegMesh(16, 0.0, 1.0)  
print(mesh.ps())  
print(mesh.ws())
```

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Numerical integration

On-shell singularity

- consider now Eq. (10) written out and with explicit expression for G_0
- assume furthermore we have projected the equation on a single fixed partial wave:

$$T(E_k + i\varepsilon; p, k) = V(p, k) + \int_0^\Lambda \frac{dq q^2}{2\pi^2} \frac{V(p, q)T(E_k + i\varepsilon; q, k)}{k^2 + i\varepsilon - q^2} \quad (14)$$

- for convenience, we have introduced a momentum cutoff Λ
- for $\varepsilon = 0$, we would be integrating over the **singularity at $q = p$** , which can be isolated by writing

$$k^2 + i\varepsilon - q^2 = -(q - k - i\tilde{\varepsilon})(q + k), \quad (15)$$

where $\lim_{\tilde{\varepsilon} \rightarrow 0}$ is equivalent to $\lim_{\varepsilon \rightarrow 0}$

- this can now be dealt with using the **principal value formula**

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{x \pm i\varepsilon} = \text{PV} \frac{1}{x} \mp i\pi\delta(x) \quad (16)$$

- but how do we realize this with a numerical quadrature?

Numerical principal value integration

- schematically we are dealing with an integral of the form

$$\lim_{\varepsilon \rightarrow 0} \int_0^\Lambda dq \frac{f(q)}{q - (k + i\varepsilon)} = \text{PV} \int_0^\Lambda dq \frac{f(q)}{q - k} + i\pi f(k) \quad (17)$$

where we have defined

$$f(q) = -\frac{q^2}{2\pi^2} \frac{V(p, q)T(E_k; q, k)}{q + k} \quad (18)$$

- now, we add $0 = f(k) - f(k)$ in Eq. (17) and get:

$$\text{PV} \int_0^\Lambda dq \frac{f(q) - f(k)}{q - k} + \text{PV} \int_0^\Lambda dq \frac{f(k)}{q - k} \quad (19)$$

- in the first term, the numerator **cancels the singularity**
- the integral in the second term can be **solved analytically**

Numerical principal value integration

- overall, we have arrived at

$$\text{PV} \int_0^\Lambda dq \underbrace{\frac{f(q) - f(k)}{q - k}}_{\tilde{f}(q)} + \text{PV} \int_0^\infty dq \frac{f(k)}{q - k} + i\pi f(k) \quad (20)$$

- ▶ to the first term, we can now apply a standard quadrature: $\rightarrow \sum w_i \tilde{f}(q_i)$
 - ▶ after this step, we can **split up \tilde{f} again** because it's all finite sums!
 - ▶ the second term is simply $f(k) \log\left(\frac{\Lambda - k}{k}\right)$
- eventually, we arrive at the original integral (first part of \tilde{f}), and a sum of three terms multiplying $f(k)$:

$$R = \sum_i \frac{w_i}{q_i - k} + \log\left(\frac{\Lambda - k}{k}\right) + i\pi \quad (21)$$

- this can be interpreted as **adding an additional point $q_0 = k$** with **weight $w_0 = R$** to the original quadrature mesh $\{q_i\}_{i=1}^N$

Partial-wave projection

- for V spherically symmetric, it makes sense to expand the T-matrix in partial waves:

$$T(E_{\mathbf{k}}; \mathbf{p}, \mathbf{k}) = \sum_{l=0}^{\infty} (2l+1) T_l(E_k; p, k) P_l(\cos \theta) \quad (22)$$

- $\cos \theta$ here denotes the angle between \mathbf{k} and \mathbf{p}
- the l -th **partial-wave projection** is then given by

$$T_l(E_k; p, k) = \frac{1}{2} \int d \cos \theta P_l(\cos \theta) T(E_{\mathbf{k}}; \mathbf{p}, \mathbf{k}) \quad (23)$$

- this projection can be applied to the Lippmann-Schwinger equation as a whole:

$$T_l(E_k + i\varepsilon; p, k) = V_l(p, k) + \int \frac{dq q^2}{2\pi^2} V_l(p, q) G_0(E_k + i\varepsilon; q) T_l(E_k + i\varepsilon; q, k) \quad (24)$$

- this involves the **partial-wave projected potential** $V_l(p, k)$

Scattering amplitude

- the **scattering amplitude** is now defined, for $|\mathbf{k}'| = |\mathbf{k}| = k$, as

$$f(\mathbf{k}', \mathbf{k}) = f_k(\theta) = -\frac{\mu}{2\pi} \langle \mathbf{k}' | V | \psi_{\mathbf{k}}^{(+)} \rangle = -\frac{\mu}{2\pi} \langle \mathbf{k}' | T | \mathbf{k} \rangle \quad (25)$$

- physically, it describes the **modulation of the outgoing scattered wave**
- it has an expansion into partial waves analogous to the T-matrix
- the **on-shell T-matrix** is related to the partial-wave scattering amplitude, and also to the **partial-wave S-matrix**

$$f_l(k) = -\frac{\mu}{2\pi} T_l(E_k; k, k) = \frac{S_l(k) - 1}{2ik} \quad (26)$$

Notes

- conventions regarding the prefactors in Eq. (26) may differ in the literature
- in the three-dimensional vector representation, the **on-shell point** is defined as $T(E_{\mathbf{k}}; \mathbf{k}', \mathbf{k})$ with $|\mathbf{k}'| = |\mathbf{k}|$, leaving a dependence on θ

Scattering phase shift

- **unitarity** of the partial-wave S-matrix, $|S_l(k)| = 1$, implies that

$$S_l(k) = e^{2i\delta_l(k)} \quad (27)$$

- this defines the **scattering phase shift** $\delta_l(k)$
- the factor of two in the exponent is a (convenient) convention at this point
- from this form we obtain further useful ways to express the scattering amplitude:

$$f_l(k) = \frac{e^{2i\delta_l(k)} - 1}{2ik} = \frac{e^{i\delta_l(k)} \sin \delta_l(k)}{k} = \frac{1}{k \cot \delta_l(k) - ik} \quad (28)$$

- the final form in Eq. (28) is particularly useful to **calculate the phase shift from the T-matrix**:

$$\delta_l(k) = \operatorname{arccot} \left(-\frac{2\pi}{\mu k} T(E_k; k, k)^{-1} + i \right) \quad (29)$$

- the ik in the Eq. (28) is directly related to the $i\pi$ in the principal-value formula

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Solution of Lippmann-Schwinger equation

Effective range expansion

- the scattering amplitude can be expanded in p , and it can be shown that for the l -th partial wave, $f_l(k) = \mathcal{O}(k^{2l})$, so:

$$f_l(p) = \frac{1}{k \cot \delta_l(k) - ik} = \sum_{n=2l}^{\infty} c_{l,n} k^n \quad (30)$$

- this implies a **hierarchy of partial waves**
 - larger l become subsequently important as k increases
 - only S-waves ($l = 0$) contribute for $k \rightarrow 0$
- odd powers in Eq. (30) actually only arise from the **unitarity cut**, $-ik$
- all nontrivial physics information is contained in $k \cot \delta_l(k)$, and this quantity is **analytic in $k^2 \sim E$**
- conventionally one defines the **effective range expansion** as

$$k^{2l+1} \cot \delta_l(k) = -\frac{1}{a_l} + \frac{r_l}{2} k^2 + \mathcal{O}(k^4) \quad (31)$$

- from this one can infer that $c_{l,0} = a_l$

Scattering wavefunctions

- from the **half off-shell T-matrix**, we can also obtain **scattering wavefunctions** in momentum space
- recall the initial form of the Lippmann-Schwinger equation, Eq. (8):

$$|\psi_{\mathbf{k}}^{(+)}\rangle = |\mathbf{k}\rangle + (E_{\mathbf{k}} - H_0 + i\varepsilon)^{-1} V |\psi_{\mathbf{k}}^{(+)}\rangle$$

- with $V|\psi_{\mathbf{k}}^{(+)}\rangle = T|\mathbf{k}\rangle$, we obtain directly:

$$\langle \mathbf{q} | \psi_{\mathbf{k}}^{(+)} \rangle = \langle \mathbf{q} | \mathbf{k} \rangle + \langle \mathbf{q} | (E_{\mathbf{k}} - H_0 + i\varepsilon)^{-1} T | \mathbf{k} \rangle \quad (32)$$

- from the first term $\langle \mathbf{q} | \mathbf{k} \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{k})$ it is clear that this is a **distribution**, not an ordinary function
- the second term, with $\varepsilon \rightarrow 0$ implied, contains a **smooth part** as well as a **pole contribution** (from the on-shell point):

$$\langle \mathbf{q} | (E_{\mathbf{k}} - H_0 + i\varepsilon)^{-1} T | \mathbf{k} \rangle = \frac{2\mu T(E_{\mathbf{k}}; \mathbf{q}, \mathbf{k})}{\mathbf{k}^2 - \mathbf{q}^2 + i\varepsilon} \quad (33)$$

Scattering wavefunctions

- altogether we have

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{q}) = \langle \mathbf{q} | \psi_{\mathbf{k}}^{(+)} \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{k}) + \frac{2\mu T(E_{\mathbf{k}}; \mathbf{q}, \mathbf{k})}{\mathbf{k}^2 - \mathbf{q}^2 + i\varepsilon} \quad (34)$$

- Fourier-transform yields **wavefunctions in configuration space**:

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + 2\mu \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q} \cdot \mathbf{r}} \frac{T(E_{\mathbf{k}}; \mathbf{q}, \mathbf{k})}{\mathbf{k}^2 - \mathbf{q}^2 + i\varepsilon} \quad (35)$$

Notes

- this $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ is an **ordinary function**, but it is still not normalizable and therefore not an element of the Hilbert space $L^2(\mathbb{R}^3)$
- the integral in Eq. (35) goes across the pole at $\mathbf{q} = \mathbf{k}$, so it is again defined as a **principal value**
- numerically this is handled by exactly the same **modified quadrature rule** as before

Scattering eigenstates

- the Schrödinger equation asserts that

$$(H_0 + V)|\psi_{\mathbf{k}}^{(+)}\rangle = E_p|\psi_{\mathbf{k}}^{(+)}\rangle \quad (36)$$

- in configuration space, where $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ is an ordinary function and H is a differential operator, we can test this by looking at the **ratio** $(H\psi_{\mathbf{k}}^{(+)})(\mathbf{r})/\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$
- in momentum space, the analog of this is not well defined because we are dealing with **distributions**:

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{q}) = (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{k}) + \dots \quad (37)$$

- nor can we take matrix elements of $|\psi_{\mathbf{k}}^{(+)}\rangle$
- the resolution is that scattering states are really **generalized eigenstates** of the Hamiltonian, in the sense that for any **test function** $\phi(\mathbf{q}) = \langle\phi|\mathbf{q}\rangle$ it holds that

$$\langle\phi|(H_0 + V)|\psi_{\mathbf{k}}^{(+)}\rangle = E_k \langle\phi|\psi_{\mathbf{k}}^{(+)}\rangle \quad (38)$$

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Eigenstate verification

Bound states

- we will formally derive later that bound states correspond to **poles of the S-matrix** at negative energies
- since, schematically, $S = \mathbf{1} + T$, these poles really need to be in the T-matrix
- moreover, it can be shown that these poles are necessarily **simple poles**
- therefore, assuming the existence of a bound state at energy $E = -B$, we can parametrize the T-matrix in the vicinity of the pole as follows:

$$T(E; p, p') \sim \frac{Z(p, p')}{E + B} \quad \text{for } E \rightarrow -B \quad (39)$$

- finally, it can be shown that the residue $Z(p, p')$ factorizes: $Z(p, p') = B^*(p)B(p')$
- we call $B(p)$ the **vertex fuction** associated with the bound state, and we will later derive its relation to the **momentum-space wavefunction** of the bound state
- in abstract operator notation, we write Eq. (39) as

$$T(E) \sim \frac{|B\rangle\langle B|}{E + B} \quad \text{for } E \rightarrow -B \quad (40)$$

Bound-state equation

- inserting the **factorized pole form** into the Lippmann-Schwinger equation gives:

$$\frac{B^*(p)B(p')}{E+B} = V(p, p') + \int \frac{dq q^2}{2\pi^2} V(p, q) G_0(E; q) \frac{B^*(q)B(p')}{E+B} \quad (41)$$

- we have used here the partial-wave projected form and dropped the subscript l
- next, we multiply through with $(E+B)$ and **take the limit $E \rightarrow -B$**
 - the potential does not have any poles, so $\lim_{E \rightarrow -B} V(p, p') = 0$
 - the free Green's function is also regular for $E < 0$

$$B^*(p)B(p') = \int \frac{dq q^2}{2\pi^2} V(p, q) G_0(-B; q) B^*(q)B(p') \quad (42)$$

- finally, we can drop the common factor $B(p')$ on both sides and use that both V and G_0 are real to obtain the **Schrödinger equation for the vertex function**:

$$B(p) = \int \frac{dq q^2}{2\pi^2} V(p, q) G_0(-B; q) B(q) \quad (43)$$