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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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:

• all physics information is contained in the scattering amplitude $f_k(heta)$

Free Hamiltonian

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

$$H_0 |\mathbf{k}
angle = rac{\mathbf{k}^2}{2\mu} |\mathbf{k}
angle$$

▶ this is for a two-body system with relative momentum **k** and reduced mass μ

Note

- the plane-wave states ${\bf k}$ are not elements of the physical Hilbert space

1

- $\langle {f r} | {f k}
 angle = {
 m e}^{{
 m i} {f k} \cdot {f r}}$ is not a normalizable wavefunction ($ot\in L^2({\mathbb R}^3)$)
- strictly one should work with wave packets $|\phi
 angle\sim\int\mathrm{d}^3p\,g(\mathbf{p})|\mathbf{p}
 angle$
- 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:

$$V({f r}',{f r})=\langle {f r}'|V|{f r}
angle$$

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

$$V_l(p',p) = 4\pi \int_0^\infty \mathrm{d}r \, r^2 j_l(p'r) V(r) j_l(pr) \,,$$
 (3)

where $j_l(z)$ it 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

$$V_l(p',p) = rac{4\pi}{p'p} \int_0^\infty \mathrm{d}r \, \hat{j}_l(p'r) V(r) \hat{j}_l(pr)$$
 (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: $H|\psi
 angle=E|\psi
 angle$ with $H=H_0+V$
- this equation alone does not specify a boundary condtion for solutions $\psi({f r})=\langle {f r}|\psi
 angle$
- a scattering state should be such that for V o 0 , $|\psi
 angle o |{f k}
 angle$
- moreover, the state should be one that evolved from a free state in the infinite past

Interlude: time dependence

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

$$G_0(t) = G_0^{(+)}(t) = egin{cases} -\mathrm{i} \mathrm{e}^{-\mathrm{i} H_0 t} & t > 0\,, \ 0 & t \leq 0 \ \end{cases}$$
 (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:

$$|\psi_{\mathrm{in}}(t)
angle = \lim_{t'
ightarrow -\infty}\mathrm{i}G_{0}^{(+)}(t-t')|\psi(t')
angle \tag{6}$$

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

$$|\psi(t)
angle = |\psi_{
m in}(t)
angle + \lim_{arepsilon
ightarrow 0^+}\int {
m d}t\,{
m e}^{-arepsilon t'}G^{(+)}(t-t')V|\psi_{
m in}(t)
angle \tag{7}$$

- if the states monochromatic (fixed definite energy), the damping factor $e^{-\varepsilon t'}$ with $\varepsilon \to 0^+$ is required in Eq. (7)
- approximately this can be interpreted as multiplying the potential V with $e^{-\varepsilon t'}$, adibatically 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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- moreover, the state should be one that evolved from a free state in the infinite past
- both conditions can be enforced with the ansatz

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

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

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

Notes

- free Green's function $G_0(z)=(z-H_0)^{-1}$ appears in Eq. (8) with $z=E_{f k}+{
 m i}arepsilon$
- arepsilon
 ightarrow 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:

$$V|\psi_{\mathbf{k}}^{(+)}
angle = V|\mathbf{k}
angle + VG_0(E_{\mathbf{k}} + \mathrm{i}arepsilon)V|\psi_{\mathbf{k}}^{(+)}
angle$$

$$\tag{9}$$

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

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

this represents the Lippmann-Schwinger equation for the operator T

Notes

- since **k** is arbitrary in Eq. (10), we postulate at the operator level: $T = V + VG_0T$
- $T = T(E_{\mathbf{k}} + \mathrm{i}\varepsilon)$ 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 $\langle {\bf p}|$ from the left and define $T(E_{\bf k}+{\rm i}\varepsilon;{\bf p},{\bf k})=\langle {\bf p}|T(E_{\bf k}+{\rm i}\varepsilon)|{\bf k}\rangle$
- this is called the **T-matrix**, and it satisfies

$$\langle \mathbf{p}|T|\mathbf{k}\rangle = \langle \mathbf{p}|V|\mathbf{k}\rangle + \langle \mathbf{p}|VG_0(E_\mathbf{k} + \mathrm{i}\varepsilon)T|\mathbf{k}\rangle \tag{11}$$

- Eq. (11) involves the momentum-space potential $V({f p},{f k})=\langle {f p}|V|{f k}
 angle$
- 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: $\langle {f q}|G_0(z)|{f q}'
 angle = G_0(z;{f q})\delta^{(3)}({f q}-{f q}')$

 $T(E_{f k}+{
m i}arepsilon;{f p},{f k})=V({f p},{f k})$

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

• 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

$$\int_{a}^{b} f(p) \,\mathrm{d}p \approx \sum_{i=1}^{N} w_i f(p_i) \tag{13}$$

- 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:

$$T(E_k + \mathrm{i}arepsilon; p, k) = V(p, k) + \int_0^{\Lambda} rac{\mathrm{d}q \, q^2}{2\pi^2} rac{V(p, q)T(E_k + \mathrm{i}arepsilon; q, k)}{k^2 + \mathrm{i}arepsilon - q^2}$$
(14)

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

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

where $\lim_{ ilde{arepsilon}
ightarrow 0}$ is equivalent to $\lim_{arepsilon
ightarrow 0}$

• this can now be dealt with using the principal value formula

$$\lim_{\varepsilon \to 0} \frac{1}{x \pm \mathrm{i}\varepsilon} = \mathrm{PV}\frac{1}{x} \mp \mathrm{i}\pi\delta(x) \tag{16}$$

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

Numerical principal value integration

• schematically we are dealing with an integral of the form

$$\lim_{\varepsilon \to 0} \int_0^{\Lambda} \mathrm{d}q \, \frac{f(q)}{q - (k + \mathrm{i}\varepsilon)} = \mathrm{PV} \int_0^{\Lambda} \mathrm{d}q \, \frac{f(q)}{q - k} + \mathrm{i}\pi f(k) \tag{17}$$

where we have defined

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

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

$$\operatorname{PV} \int_0^{\Lambda} \mathrm{d}q \, \frac{f(q) - f(k)}{q - k} + \operatorname{PV} \int_0^{\Lambda} \mathrm{d}q \, \frac{f(k)}{q - k} \tag{19}$$

- ▶ 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

$$\operatorname{PV} \int_{0}^{\Lambda} \mathrm{d}q \underbrace{\frac{f(q) - f(k)}{q - k}}_{\tilde{f}(q)} + \operatorname{PV} \int_{0}^{\infty} \mathrm{d}q \frac{f(k)}{q - k} + \mathrm{i}\pi f(k)$$
(20)

- ullet to the first term, we can now apply a standard quadrature: $ightarrow \sum w_i ilde{f}\left(q_i
 ight)$
- 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):

$$R = \sum_{i} rac{w_i}{q_i - k} + \log igg(rac{\Lambda - k}{k} igg) + \mathrm{i} \pi$$
 (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:

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

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

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

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

$$egin{aligned} T_l(E_k+\mathrm{i}arepsilon;p,k) &= V_l(p,k) \ &+ \int rac{dq\,q^2}{2\pi^2} V_l(p,q) G_0(E_k+\mathrm{i}arepsilon;q) T_l(E_k+\mathrm{i}arepsilon;q,k) \end{aligned}$$

• 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

$$f(\mathbf{k}',\mathbf{k}) = f_k(heta) = -rac{\mu}{2\pi} \langle \mathbf{k}' | V | \psi_{\mathbf{k}}^{(+)}
angle = -rac{\mu}{2\pi} \langle \mathbf{k}' | T | \mathbf{k}
angle$$
 (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

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

$$S_l(k) = \mathrm{e}^{2\mathrm{i}\delta_l(k)}$$
 (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:

$$f_l(k) = rac{\mathrm{e}^{\mathrm{2\mathrm{i}}\delta_l(k)}-1}{\mathrm{2\mathrm{i}}k} = rac{\mathrm{e}^{\mathrm{i}\delta_l(k)}\sin\delta_l(k)}{k} = rac{1}{k\cot\delta_l(k)-\mathrm{i}k}$$

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

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

• the ik in the Eq. (28) is directly related to the i π 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:

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

- this implies a hierarchy of partial waves
 - larger l become subsequently important as k increases
 - \blacktriangleright only S-waves (l=0) contribute for k
 ightarrow 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

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

$$|\psi^{(+)}_{\mathbf{k}}
angle = |\mathbf{k}
angle + (E_{\mathbf{k}}-H_0+\mathrm{i}arepsilon)^{-1}V|\psi^{(+)}_{\mathbf{k}}
angle$$

• with $V|\psi^{(+)}_{f k}
angle=T|{f k}
angle$, we obtain directly:

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

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

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

Scattering wavefunctions

• altogether we have

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

• Fourier-transform yields wavefunctions in configuration space:

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

$$(H_0+V)|\psi^{(+)}_{\mathbf{k}}
angle=E_p|\psi^{(+)}_{\mathbf{k}}
angle$$
 (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:

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

- nor can we take matrix elements of $|\psi^{(+)}_{f k}
 angle$
- 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

$$\langle \phi | (H_0 + V) | \psi_{\mathbf{k}}^{(+)}
angle = E_k \langle \phi | \psi_{\mathbf{k}}^{(+)}
angle$$
 (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:

$$T(E;p,p') \sim rac{Z(p,p')}{E+B} \ ext{for} \ E
ightarrow -B$$
 (39)

- finally, it can be shown that the residue $Z(p,p^\prime)$ factorizes: $Z(p,p^\prime)=B^*(p)B(p^\prime)$
- 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

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

Bound-state equation

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

$$\frac{B^*(p)B(p')}{E+B} = V(p,p') + \int \frac{dq \, q^2}{2\pi^2} V(p,q) G_0(E;q) \frac{B^*(q)B(p')}{E+B}$$
(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
 ightarrow -B
 - the potential does not have any poles, so $\lim_{E
 ightarrow -B}V(p,p')=0$
 - \blacktriangleright the free Green's function is also regular for E < 0

$$B^{*}(p)B(p') = \int \frac{\mathrm{d}q \, q^{2}}{2\pi^{2}} V(p,q)G_{0}(-B;q)B^{*}(q)B(p') \tag{42}$$

• 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:

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