

M1b. Scattering Theory 1

a. To be covered in Scattering Theory 2 (T1b)

This is a non-exhaustive list of what will be covered in T1b.

- Electromagnetic part of the NN interaction
- Bound states and NN scattering
 - basic deuteron properties (but not mixing)
 - absence of other two-body bound states
- Phenomenology of NN phase shifts (e.g., à la Machleidt)
 - Both S-waves and large scattering lengths. Effective range effects. Sign changes
 - what parts of forces contribute to different phases
 - low vs. high L partial waves
- How high in energy and partial wave and how accurately do phase shifts need to be reproduced for various nuclear applications?

b. Reminder of basic quantum mechanical scattering

Our first and dominant source of information about the two-body force between nucleons (protons and neutrons) is nucleon-nucleon scattering. All of you are familiar with the basic quantum mechanical formulation of non-relativistic scattering. We will review and build on that knowledge in this lecture and the exercises.

Nucleon-nucleon scattering means n - n , n - p , and p - p . While all involve electromagnetic interactions as well as the strong interaction, p - p has to be treated specially because of the Coulomb interaction (what other electromagnetic interactions contribute to the other scattering processes?). We'll start here with neglecting the electromagnetic potential V_{em} and the difference between the proton and neutron masses (this is a good approximation, because $(m_n - m_p)/m \approx 10^{-3}$ with $m \equiv (m_n + m_p)/2$). So we consider a generic case of scattering two particles of mass m in a short-ranged potential V . While we have in mind that $V = V_{\text{NN}}$, we won't consider those details until tomorrow's lectures.

Let's set our notation with a quick review of scattering (without derivation). The Hamiltonian (in operator form) is

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + V, \quad (1)$$

where we label the momentum operators for particles 1 and 2. We switch to relative ("rel") and

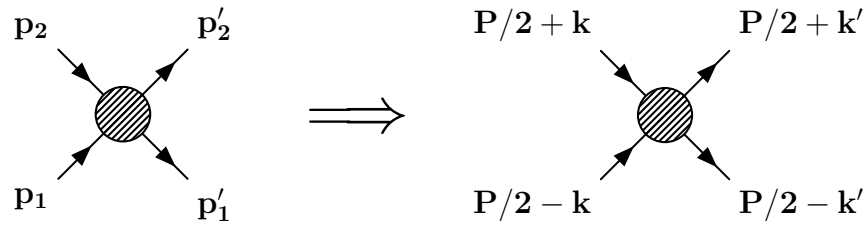


Figure 1: Kinematics for scattering in lab and relative coordinates. If these are external (and therefore “on-shell”) lines for elastic scattering, then when $\mathbf{P} = 0$ we have $k^2 = k'^2 = mE_k = 2\mu E_k$ (assuming equal masses m).

center-of-mass (“cm”) coordinates:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \tag{2}$$

$$\mathbf{k} = \frac{\mathbf{p}_1 - \mathbf{p}_2}{2}, \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \tag{3}$$

so that the Hamiltonian becomes (still operators, but the \mathbf{P} , \mathbf{k} , and \mathbf{k}' in Fig. 1 are numbers)

$$H = T_{\text{cm}} + H_{\text{rel}} = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{k}^2}{2\mu} + V, \tag{4}$$

with total mass $M = m_1 + m_2 = 2m$ and reduced mass $\mu = m_1 m_2 / M = m/2$. (Note: H_{rel} is sometimes called the intrinsic Hamiltonian.) Now we note that V depends only on the cm variables (more on this tomorrow!), which means that we can separate the total wave function into a plane wave for the center-of-mass motion (only kinetic energy) and the wave function for relative motion:

$$|\Psi\rangle = |\mathbf{P}\rangle |\psi_{\text{rel}}\rangle. \tag{5}$$

As a result, the two-body problem has become an effective one-body problem. From now on, we are only concerned with $|\psi_{\text{rel}}\rangle$, so we will drop the “rel” most of the time.

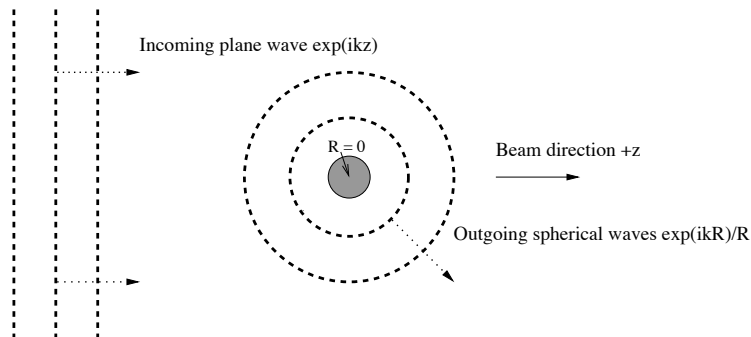


Figure 2: Scattering problem for an incident plane wave in the $+z$ direction on a spherical target (in the text r is used instead of R). [From F. Nunes notes.]

Thus we can consider relative motion with total $P = 0$ (see Fig. 1) and describe elastic scattering from a potential from incoming \mathbf{k} to outgoing \mathbf{k}' with $|\mathbf{k}| = |\mathbf{k}'|$ and $E = k^2/(2\mu)$ (with $\hbar = 1$). We describe this quantum mechanically in terms of an incoming plane wave and an outgoing scattered (“sc”) wave:

$$\psi_E^{(+)}(\mathbf{r}) = \psi_{\text{in}}(\mathbf{r}) + \psi_{\text{sc}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} + \psi_{\text{sc}}(\mathbf{r}), \quad (6)$$

which (assuming V falls off with r faster than $1/r$), means that far way from the potential the wave function has the asymptotic form

$$\psi_E^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left(e^{i\mathbf{k}\cdot\mathbf{r}} + f(k, \theta, \phi) \frac{e^{ikr}}{r} \right), \quad (7)$$

where the scattering angle θ is given by $\cos \theta = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$. A schematic picture is shown in Fig. 2 with $\mathbf{k} = k\hat{z}$. The scattering amplitude f modulates the outgoing spherical wave according to direction and carries all the physics information.

The differential cross section is calculated from

$$\frac{d\sigma}{d\Omega}(k, \theta, \phi) = \frac{\text{number of particles scattering into } d\Omega \text{ per unit time}}{\text{number of incident particles per unit area and time}} = \frac{S_{\text{sc},r} r^2}{S_{\text{in}}}, \quad (8)$$

where $S_{\text{sc},r}$ and S_{in} are the scattered and incoming probability current densities, respectively. Taking $\mathbf{k} \propto \hat{z}$ without loss of generality (and with $\hbar = 1$ and suppressing common $(2\pi)^3$ factors),

$$S_{\text{in}} = \text{Re} \left(\psi_{\text{in}}^* \frac{1}{i\mu} \frac{d}{dz} \psi_{\text{in}} \right) = \text{Re} \left(e^{-ikz} \frac{1}{i\mu} ik e^{ikz} \right) \propto \frac{k}{\mu}, \quad (9)$$

$$S_{\text{sc},r} = \text{Re} \left(\psi_{\text{sc}}^* \frac{1}{i\mu} \frac{d}{dr} \psi_{\text{sc}} \right) = \text{Re} \left(f^* \frac{e^{-ikr}}{r} \frac{1}{i\mu} ik f \frac{e^{ikr}}{r} \right) + \mathcal{O} \left(\frac{1}{r^3} \right) \propto \frac{k}{\mu r^2} |f|^2 + \mathcal{O} \left(\frac{1}{r^3} \right), \quad (10)$$

so the differential cross section is

$$\frac{d\sigma}{d\Omega}(k, \theta, \phi) = |f(k, \theta, \phi)|^2. \quad (11)$$

If we do not consider spin observables (where the spin orientation of at least one of the particles is known—polarized), then $f(k, \theta, \phi)$ is independent of ϕ ; we consider only this case for now and drop the ϕ dependence.

We expand the wave function in spherical coordinates as

$$\psi(r, \theta) = \sum_{l=0}^{\infty} c_l \frac{u_l(r)}{r} Y_{l0}(\theta, \phi) = \sum_{l=0}^{\infty} \tilde{c}_l \frac{u_l(r)}{r} P_l(\cos \theta), \quad (12)$$

where because there is no ϕ dependence, only the $m_l = 0$ spherical harmonic $Y_{l0}(\theta, \phi) = \langle \theta, \phi | l, m_l = 0 \rangle$ appears and we can use $Y_{l0} = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta)$. The radial function $u_l(r)$ satisfies the radial Schrödinger equation (if there is no mixing of different l values),

$$\frac{d^2 u_l}{dr^2} - \left(\frac{l(l+1)}{r^2} + 2\mu V - k^2 \right) u_l(r) = 0. \quad (13)$$

We have freedom in choosing the normalization of u_l , which we will exploit below.

For a central potential V (we'll come back to non-central potentials tomorrow!), we resolve the scattering amplitude f into decoupled partial waves (the definition of f_l sometimes has a extra k factor):

$$f(k, \theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos \theta). \quad (14)$$

[We can do a partial wave expansion even if the potential is not central, which means the potential does not commute with the *orbital* angular momentum (as in the nuclear case!); it merely means that different l 's will mix to some degree (in the nuclear case, this includes triplet S and D waves). The more important question is how many total l 's do we need to include to ensure convergence of observables of interest.] Using the plane wave expansion of the incoming wave,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) \xrightarrow{r \rightarrow \infty} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \frac{(-1)^{l+1} e^{-ikr} + e^{ikr}}{2ikr}, \quad (15)$$

where we have used the asymptotic form of the spherical Bessel function j_l :

$$j_l(kr) \xrightarrow{r \rightarrow \infty} \frac{\sin(kr - l\frac{\pi}{2})}{kr} = \frac{1}{kr} \frac{(-i)^l e^{ikr} - i^l e^{-ikr}}{2i}, \quad (16)$$

we can resolve the asymptotic wave function into incoming (e^{-ikr}) and outgoing (e^{ikr}) spherical waves (so now effectively a one-dimensional interference problem):

$$\psi_E^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \frac{(-1)^{l+1} e^{-ikr} + S_l(k) e^{ikr}}{2ikr}, \quad (17)$$

which identifies the partial wave S-matrix

$$S_l(k) = 1 + 2ik f_l(k). \quad (18)$$

[Note: in scattering theory you will encounter many closely related functions with different normalizations, often defined just for convenience and/or historical reasons. Be careful that you use consistent conventions!] So part of e^{ikr} is the initial wave and part is the scattered wave; the latter defines the scattering amplitude, which is proportional to the on-shell T-matrix (see below). The conservation of probability for elastic scattering implies that $|S_l(k)|^2 = 1$ (the S-matrix is unitary).

The real phase shift $\delta_l(k)$ is introduced to parametrize the S-matrix:

$$S_l(k) = e^{2i\delta_l(k)} = \frac{e^{i\delta_l(k)}}{e^{-i\delta_l(k)}}, \quad (19)$$

(the second equality is a trivial consequence but nevertheless is useful in manipulating scattering equations) which leads us to write the partial-wave scattering amplitude f_l as

$$f_l(k) = \frac{S_l(k) - 1}{2ik} = \frac{e^{i\delta_l(k)} \sin \delta_l(k)}{k} = \frac{1}{k \cot \delta_l(k) - ik}. \quad (20)$$

We will see the combination $k \cot \delta_l$ many times. Putting things together, the asymptotic wave function can be written (suppressing the k dependence of δ_l):

$$\psi_E^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) i^l e^{i\delta_l} \frac{\sin(kr - l\frac{\pi}{2} + \delta_l)}{kr}, \quad (21)$$

where the “shift in phase” is made manifest. Two pictures that go with this phase shift are shown in Fig. 3. From above, the total cross section is

$$\sigma(k) = 4\pi \sum_{l=0}^{\infty} (2l+1) |f_l(k)|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k). \quad (22)$$

Note that there is an ambiguity in δ_l because we can change it by adding multiples of π without changing the physics. If we specify that the phase shift is to be continuous in k and that it goes to zero as $k \rightarrow \infty$ (that is, that $\delta_l(\infty) = 0$), then we remove the ambiguity and Levinson’s theorem holds:

$$\delta_l(k=0) = n_l \pi, \quad (23)$$

where n_l is the number of bound states in the l^{th} partial wave. [This is sometimes given alternatively as $\delta_l(0) - \delta_l(\infty) = n_l \pi$.]

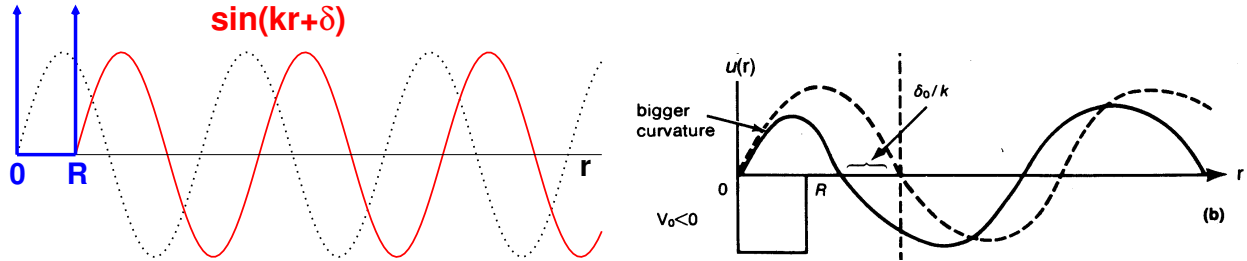


Figure 3: Repulsive and attractive phase shifts. On the left is an extreme example: a repulsive “hard sphere”. The figure on the right is from a textbook on quantum mechanics, but note how crude the figure is: the phase shift doesn’t stay the same for $r > R$!

An easy (but somewhat pathological) case to consider is hard-sphere scattering, for which there is an infinitely repulsive wall at $r = R$. (You can think of this as a caricature of a strongly repulsive short-range potential — a “hard core”.) Since the potential is zero outside of R and the wave function must vanish in the interior of the potential (so that the energy is finite), we can trivially write down the S -wave scattering solution for momentum k : it is just proportional to a sine function shifted by kR from the origin, $\sin(kr - kR)$. Thus the phase shift is

$$\delta_0(k) = -kR \text{ [for a hard sphere]}. \quad (24)$$

It will be convenient to use this as a test case in talking about the effective range expansion and pionless EFT in free space and at finite density. (Note that the hard sphere is not really a potential but a boundary condition on the wave function; e.g., we can’t use the VPA (see below) for $r < R$. We can’t choose the phase shift to vanish at high energy, either, unless we make the repulsion very

large but not infinite — then the VPA says it will vanish because of the $1/k$ factor on the right side. Does Levinson’s theorem hold anyway?)

More details on scattering at this level can be found in (practically) any first-year graduate quantum mechanics text. For a more specialized (but very readable) account of nonrelativistic scattering, check out “Scattering Theory” by Taylor. For all the mathematical details and thorough coverage, see the book by Newton.

c. Computational methods for phase shifts: Variable Phase Approach

c.1 “Conventional” way to solve for phase shifts in coordinate representation

In coordinate space, one can use the basic definition of phase shifts to carry out a numerical calculation. In particular, for a given (positive) energy, the Schrödinger equation can be integrated out from the origin using a differential equation solver (such as those built into Mathematica and MATLAB or readily available for other languages) until the asymptotic region ($r \gg R$, where R is the “range” of the potential — how do you know how far?). At that point one uses the asymptotic form (for partial wave l with $\hat{j}_l(z) \equiv z * j_l(z)$ and $\hat{n}_l(z) \equiv z * n_l(z)$)

$$u_l(r) \xrightarrow{r \rightarrow \infty} \cos \delta_l(k) \hat{j}_l(kr) - \sin \delta_l(k) \hat{n}_l(kr) , \quad (25)$$

to identify $\delta_l(k)$. To check: the S -wave ($l = 0$) phase shift is

$$u_0(r) \xrightarrow{r \rightarrow \infty} \sin[kr + \delta_0(k)] = \cos \delta_0 \sin kr + \sin \delta_0 \cos kr . \quad (26)$$

(Recall that $\hat{j}_0(z) = \sin z$ and $\hat{n}_0(z) = -\cos z$.) At a given point r_1 , Eq. (25) has two unknowns, $\cos \delta_l$ and $\sin \delta_l$, so we need two equations to work with. Two ways to get them and extract δ_l are:

1. calculate at two different points $u(r_1)$ and $u(r_2)$, form $u(r_1)/u(r_2)$ and then solve for $\tan \delta(k)$;
2. calculate $u(r_1)$ and $u'(r_1)$, take the ratio and then solve for $\tan \delta$.

Either way works fine numerically if you have a good differential equation solver (for which you can specify error tolerances).

c.2 Basics of the VPA

As just described, we can solve for the phase shifts by integrating the Schrödinger equation numerically in r from the origin, using any normalization we want. As we proceed, the end effect on the phase shift of a local potential up to any given radius is completely determined once the integration reaches that point (it is a *local* effect for a local potential). In response to the potential the wave function is either pulled in with each step in r (when attractive) or pushed out (when repulsive) and this information must be accumulated during the integration. So we should be able to devise an alternative method that simply builds up the phase shift directly as an integration from $r = 0$ to outside of the range of the potential.

This alternative method is the Variable Phase Approach (VPA). Here is the basic idea for the $l = 0$ partial wave for a local potential $V(r)$. Generalizations exist for higher partial waves (a problem for you!) and for non-local potentials (more complicated but interesting; [add refs!]). We introduce the potential $V_\rho(r)$, which agrees with $V(r)$ out to $r = \rho$ and then is zero:

$$V_\rho(r) = \begin{cases} V(r) & r \leq \rho \\ 0 & r > \rho \end{cases} \quad (27)$$

Now we'll consider the "regular solution" $\phi(r)$, which is different from the conventional scattering solution only by its normalization, which is chosen so that $\phi(r) \xrightarrow{r \rightarrow 0} \sin(kr)$, with no other multiplicative factors: $\phi(0) = 0$, $\phi'(0) = 1$.

[Aside on regular solutions versus ordinary normalization. Typically one uses the following normalization for angular momentum l and scattering momentum p (so $E = p^2/2\mu$):

$$\int_0^\infty dr u_{l,p'}^*(r) u_{l,p}(r) = \frac{\pi}{2} \delta(p' - p) \quad (28)$$

(see AJP article equations 91a,b and 69a,b) with the two boundary conditions that

$$u_{l,p}(r=0) = 0 \quad \text{and} \quad u_{l,p}(r) \xrightarrow{r \rightarrow \infty} \hat{y}_l + p f_l \hat{h}_l^+ . \quad (29)$$

In contrast, the regular solution is defined by the *initial condition* $\phi_{l,p}(r) \xrightarrow{r \rightarrow 0} \hat{y}_l(pr)$ with no extra factors.]

Let $\phi(r)$ and $\phi_\rho(r)$ be the regular solutions for $V(r)$ and $V_\rho(r)$ with phase shifts at energy $E = k^2/2\mu$ given by $\delta(k)$ and $\delta(k, \rho)$, respectively. When there is no potential there is no phase shift (by definition), so $\delta(k, 0) = 0$. At large ρ , the potentials are the same, so

$$\delta(k, \rho) \xrightarrow{\rho \rightarrow \infty} \delta(k) , \quad (30)$$

which is the desired phase shift. This is called the "accumulation of the phase shift". The claim is that, for fixed k , the r -dependent phase shift $\delta(k, r)$ [using r instead of ρ as the variable] satisfies a first-order (nonlinear) differential equation:

$$\frac{d}{dr} \delta(k, r) = -\frac{1}{k} U(r) \sin^2[kr + \delta(k, r)] , \quad (31)$$

where $U(r) \equiv 2\mu V(r)$. Comments:

- The equation is easily integrated in practice using a differential equation solver from $r = 0$ with the initial condition $\delta(k, 0) = 0$ until the asymptotic region. It is evident when you get to this region because $\delta(k, r)$ becomes independent of r (to the needed accuracy).
- There is no multiple-of- π ambiguity in the result because we build in the conditions that the phase shift be a continuous function of k and that it vanish at high energy is built in. (Can you see how that holds?). So Levinson's theorem works (i.e., the value of the phase shift at zero energy will be $n_l \pi$, where n_l is the number of bound states). [One of the exercises is to demonstrate with numerical examples.] The case of a s-wave zero-energy bound state (or resonance) is a special case, for which we get $\pi(n_0 + 1/2)$ rather than $n_0 \pi$ at $k = 0$.

- In any partial wave, it seems sufficient to know one number at a particular radius as long as we know the potential. How can we use this?
- It is manifest that an attractive potential ($V < 0$) makes the phase shift increase positively while a repulsive potential ($V > 0$) makes the phase shift more negative. The net winner when both signs of V are present is energy dependent. E.g., for NN S-waves the phase shift changes sign with energy.
- If $V(r)$ diverges as $r \rightarrow 0$ (e.g., like Coulomb), then use $\delta'(r) \sim -(1/k)U(r) \sin^2 kr$ as $r \rightarrow 0$ to start the integration.
- For non-zero l , the equation to solve is

$$\frac{d}{dr} \delta_l(k, r) = -\frac{1}{k} U(r) [\cos \delta_l(k, r) \widehat{j}_l(kr) - \sin \delta_l(k, r) \widehat{n}_l(kr)]^2. \quad (32)$$

It is clear from the definitions of the Riccati-Bessel functions that this reduces to our previous result for $l = 0$. The derivation of Eq. (32) is a simple generalization of the $l = 0$ derivation in the next section.

- In the exercises you get to play with (and extend) a Mathematica (and iPython) notebook that implements the VPA for S-wave scattering from a square-well potential in a single short definition (after `Vsw` defines $V(r)$ for a square well with radius one and depth V_0):

```
deltaVPA[k_, V0_] := (
  Rmax = 10; (* integrate out to Rmax; just need Rmax > R for square well *)
  ans = NDSolve[
    {deltarho'[r] == -(1/k) 2 mu Vsw[r, V0] Sin[k r + deltarho[r]]^2,
     deltarho[0] == 0}, deltarho, {r, 0, Rmax}, AccuracyGoal->6,
     PrecisionGoal->6]; (* Solve equation for six digit accuracy. *)
  (deltarho[r] /. ans)[[1]] /. r -> Rmax (* evaluate result at r=Rmax *)
)
```

Try it!

- Generalizations exist for coupled-channel potentials (as in the nuclear case where S and D waves can mix; more on this later) and for non-local potentials.

c.3 Derivation for $l = 0$

Return to the regular solutions: it is evident that $\phi(r)$ and $\phi_\rho(r)$ are exactly the same for $0 \leq r \leq \rho$ (which is why we normalized them that way!). For $r > \rho$, $\phi_\rho(r)$ is in the asymptotic region, so

$$\phi_\rho(r) = \alpha(\rho) \sin[kr + \delta(k, \rho)]. \quad (33)$$

Note that at this stage the r and ρ dependence is distinct. Continuity of the wave function at $r = \rho$ means

$$\phi_\rho(\rho^-) = \phi(\rho^-) = \phi(\rho^+) = \alpha(\rho) \sin[k\rho + \delta(k, \rho)] \quad (34)$$

and for the derivative it means

$$\phi'(\rho) = k\alpha(\rho) \cos[k\rho + \delta(k, \rho)] . \quad (35)$$

But now in Eqs. (34) and (35) we have just one radial variable and the equations must hold for all ρ , so we can replace ρ by r . Next we want to get an equation that only involves $\delta(k, \rho)$ and its derivative. The natural move is to consider $\phi'(r)/\phi(r)$ to get rid of $\alpha(r)$:

$$\frac{\phi'(r)}{\phi(r)} = \frac{k \cos[kr + \delta(k, r)]}{\sin[kr + \delta(k, r)]} , \quad (36)$$

and then note that

$$\frac{d}{dr} \left[\frac{\phi'}{\phi} \right] = \frac{\phi''}{\phi} - \left(\frac{\phi'}{\phi} \right)^2 , \quad (37)$$

so we can use the Schrödinger equation for the first term on the right side and then use Eq. (36) to remove all the other ϕ dependence. After some cancellations, the result is Eq. (31). Try filling in the details and generalizing to $l \neq 0$.

d. Beyond local coordinate-space potentials

d.1 Non-uniqueness of potentials

The idea of *inverse scattering* is to start with the scattering data (e.g., from experimental measurements) and reconstruct a potential that generates that data. This problem has been studied in great detail (see Newton's scattering text). Much of the development was based on the idea of finding a *local* potential, which is the type we have considered so far. The conditions for which a unique local potential can be found are well established; for example, if the phase shifts in a given partial wave are known up to infinite energy and there are no bound states and the interaction is central (no spin dependence, tensor forces, etc.), then there is a constructive way to find a unique local potential. In the literature there are discussions on finding more general classes of potentials, but usually with the disclaimer that this spoils the problem because the result is no longer unique, and besides these potentials are unphysical. As we'll see, from the modern perspective of effective field theory and the renormalization group, the focus on finding a unique potential is misguided (beyond the fact that the NN interaction has spin dependence!). We will take *advantage* of the fact that there are an infinite number of potentials (defined in the broader sense summarized below) that are *phase equivalent* in the energy region of interest; that is, they predict the same phase shifts at low energies.

This modern spirit actually goes back a long way, with the classic reference being Ekstein [Phys. Rev. **117**, 1590 (1960)]. Here is a relevant quote:

However, there are no good reasons, either from prime principles or from phenomenological analysis to exclude “nonlocal” interactions which may be, for instance, integral operators in coordinate representation.

Ekstein derives conditions for unitary transformations that produce phase equivalent potentials and notes that “this class is so wide that one is tempted to say that ‘any reasonable’ unitary transformation leaves a given Hamiltonian within its equivalence class”. However, much of mainstream low-energy nuclear physics in subsequent years carried the implicit (and sometimes explicit) idea that one should seek *the* NN potential. We will have much to say about these ideas throughout the course (and we’ll find more than one occasion when a local potential is desirable, which brings back some of the inverse scattering discussion). For now let’s review some features of unitary transformations and discuss non-local potentials.

d.2 Unitary transformations

We will encounter unitary transformations in several different contexts:

- the evolution operator $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$ and its (non-unitary) counterpart in imaginary time $t \rightarrow -i\tau$;
- symmetry transformations such as $U = e^{-i\alpha\cdot\mathbf{G}}$ with Hermitian \mathbf{G} (when we discuss constraints on NN potentials);
- unitary transformations of Hamiltonians via renormalization group methods (or by other direct transformation methods).

Recall that a unitary transformation can be realized as unitary matrices with $U_\alpha^\dagger U_\alpha = I$ (where α is just a label for the transformation). They are often used to transform Hamiltonians with the goal of simplifying nuclear many-body problems, e.g., by making them more perturbative. If I have a Hamiltonian H with eigenstates $|\psi_n\rangle$ and an operator O , then the new Hamiltonian, operator, and eigenstates are

$$\tilde{H} = UHU^\dagger \quad \tilde{O} = UOU^\dagger \quad |\tilde{\psi}_n\rangle = U|\psi_n\rangle . \quad (38)$$

The energy is unchanged (all eigenvalues are unchanged):

$$\langle \tilde{\psi}_n | \tilde{H} | \tilde{\psi}_n \rangle = \langle \psi_n | H | \psi_n \rangle = E_n . \quad (39)$$

Furthermore, if we transform everything, matrix elements of O are unchanged:

$$O_{mn} \equiv \langle \psi_m | \hat{O} | \psi_n \rangle = (\langle \psi_m | U^\dagger) U \hat{O} U^\dagger (U | \psi_n \rangle) = \langle \tilde{\psi}_m | \tilde{O} | \tilde{\psi}_n \rangle \equiv \tilde{O}_{mn} \quad (40)$$

So for consistency, we must use O with H and $|\psi_n\rangle$ ’s but \tilde{O} with \tilde{H} and $|\tilde{\psi}_n\rangle$ ’s. Claim to consider: If the asymptotic (long distance) properties are unchanged, H and \tilde{H} are equally acceptable physically. (We will have to return to the issue of what “long distance” means!) Of course, one form of the Hamiltonian may be better for intuition or another for numerical calculations.

We need to ask: *What quantities are changed and what are unchanged by such a transformation?* We have noted that energies are not, but what about the radius or quadrupole moment of a nucleus? If they can change, how do we know what answer to compare with experiment?

d.3 Local vs. non-local potentials

When we perform a unitary transformation on a potential, it is often the case that the transformed potential is non-local, even if initially it is local. Let's review what non-local means in this context (in this section we are talking about two-body systems only). Consider the operator Hamiltonian (here \mathbf{k} is the intrinsic or relative momentum):

$$\hat{H} = \frac{\hat{\mathbf{k}}^2}{2\mu} + \hat{V} \quad (41)$$

and matrix elements of \hat{H} between the wave function $|\psi\rangle$ in coordinate space:

$$\langle\psi|\hat{H}|\psi\rangle = \int d^3r \int d^3r' \langle\psi|\mathbf{r}'\rangle \langle\mathbf{r}'|\hat{H}|\mathbf{r}\rangle \langle\mathbf{r}|\psi\rangle \quad \text{with} \quad \langle\mathbf{r}|\psi\rangle \equiv \psi(\mathbf{r}), \quad (42)$$

where $\langle\mathbf{r}'|\mathbf{r}\rangle = \delta^3(\mathbf{r}' - \mathbf{r})$. The coordinate space matrix elements of the kinetic energy and potential are

$$\langle\mathbf{r}'|\frac{\hat{\mathbf{k}}^2}{2\mu}|\mathbf{r}\rangle = \delta^3(\mathbf{r}' - \mathbf{r}) \frac{-\hbar^2\nabla^2}{2\mu}, \quad \langle\mathbf{r}'|\hat{V}|\mathbf{r}\rangle = \begin{cases} V(\mathbf{r})\delta^3(\mathbf{r}' - \mathbf{r}) & \text{if local} \\ V(\mathbf{r}', \mathbf{r}) & \text{if nonlocal} \end{cases}, \quad (43)$$

where we have implicitly defined local and non-local potentials. Remember that \mathbf{r} and \mathbf{r}' are *relative* distances (e.g., $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$). We can then contrast the familiar *local* Schrödinger equation

$$\frac{-\hbar^2\nabla^2}{2\mu}\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (44)$$

with the less familiar *non-local* Schrödinger equation (which is an integro-differential equation):

$$\frac{-\hbar^2\nabla^2}{2\mu}\psi(\mathbf{r}) + \int d^3r' V(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}') = E\psi(\mathbf{r}). \quad (45)$$

From Eq. (43) we see that a local potential is rather a special case in which the interaction is diagonal in the coordinate basis. [If we considered the one-D version of this equation with the x coordinate discretized, then V becomes a matrix with off-diagonal matrix elements. Local means explicitly diagonal in this case.] An interaction that at large distances comes from particle exchange is naturally local (see the next section) and this could be considered physical. However, at short distances, the interaction between composite objects like nucleons is certainly not required to be local. But we will encounter situations in what follows where locality is an advantage.

Note that the meaning of “local” here is different than in field theory, where even local potentials would be considered non-local unless $V(\mathbf{r}) \propto \delta^3(\mathbf{r})$ as well!

e. Momentum representation

e.1 Potentials in momentum space

Consider the same abstract Hamiltonian:

$$\hat{H} = \frac{\hat{\mathbf{k}}^2}{2\mu} + \hat{V} \quad (46)$$

but now take matrix elements of the wave function $|\psi\rangle$ in *momentum* space:

$$\langle\psi|\widehat{H}|\psi\rangle = \int d^3k \int d^3k' \langle\psi|\mathbf{k}'\rangle \langle\mathbf{k}'|\widehat{H}|\mathbf{k}\rangle \langle\mathbf{k}|\psi\rangle, \quad (47)$$

with $\langle\mathbf{k}|\psi\rangle \equiv \widetilde{\psi}(\mathbf{k})$ and $\langle\mathbf{k}'|\mathbf{k}\rangle = \delta^3(\mathbf{k}' - \mathbf{k})$. The momentum-space kinetic energy and potential are

$$\langle\mathbf{k}'|\frac{\widehat{\mathbf{k}}^2}{2\mu}|\mathbf{k}\rangle = \delta^3(\mathbf{k}' - \mathbf{k}) \frac{\hbar^2 \mathbf{k}^2}{2\mu}, \quad \langle\mathbf{k}'|\widehat{V}|\mathbf{k}\rangle = \begin{cases} V(\mathbf{k}' - \mathbf{k}) & \text{if local} \\ V(\mathbf{k}', \mathbf{k}) & \text{if nonlocal} \end{cases}, \quad (48)$$

which characterizes the difference between local and non-local potentials. Remember that \mathbf{k} and \mathbf{k}' are *relative* momenta. A key example to keep in mind of what happens to a local potential when (Fourier) transformed to momentum is the Yukawa potential:

$$\frac{e^{-m|\mathbf{r}|}}{4\pi|\mathbf{r}|} \xrightarrow{\text{F.T.}} \frac{1}{(\mathbf{k}' - \mathbf{k})^2 + m^2}, \quad (49)$$

which as advertised depends on $\mathbf{k}' - \mathbf{k}$ only. (We've suppressed all of the multiplicative factors; you'll recover them in an exercise.) So if we know from physics that the longest ranged part of the NN interaction is from pion exchange, we expect that part of the potential to be local. Note that you can show directly from the Fourier transform expression that *any* local potential will only depend on the momentum transfer $\mathbf{k}' - \mathbf{k}$ [this is an exercise].

The momentum-space partial wave expansion of the potential is

$$\langle\mathbf{k}'|\widehat{V}|\mathbf{k}\rangle = \frac{2}{\pi} \sum_{l,m} V_l(k', k) Y_{lm}^*(\Omega_{k'}) Y_{lm}(\Omega_k) = \frac{1}{2\pi^2} \sum_l (2l+1) V_l(k', k) P_L(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'), \quad (50)$$

where we are using (see the Landau appendix)

$$|\mathbf{k}\rangle = \sqrt{\frac{2}{\pi}} \sum_{l,m} Y^*(\Omega_k) |klm\rangle, \quad (51)$$

which implies the completeness relation

$$1 = \frac{2}{\pi} \sum_{l,m} \int dk k^2 |klm\rangle \langle klm|. \quad (52)$$

Note that rotational invariance implies

$$\langle k'l'm'|V|klm\rangle = \delta_{ll'} \delta_{mm'} V_l(k', k). \quad (53)$$

If we start with a local potential $V(r)$, then

$$V_l(k', k) = \frac{1}{k'k} \int_0^\infty dr \widehat{j}(k'r) V(r) \widehat{j}(kr) = \int_0^\infty r^2 dr j_l(kr) V(r) j_l(k'r). \quad (54)$$

We describe momentum space scattering in terms of the T-matrix, which satisfies the Lippmann-Schwinger (LS) integral equation:

$$T^{(+)}(\mathbf{k}', \mathbf{k}; E) = V(\mathbf{k}', \mathbf{k}) + \int d^3q \frac{V(\mathbf{k}', \mathbf{q}) T(\mathbf{q}, \mathbf{k}; E)}{E - \frac{q^2}{m} + i\epsilon}, \quad (55)$$

with the partial-wave version [$T_l(k, k')$ has the same partial-wave expansion as $V_l(k, k')$ in Eq. (50)]:

$$T_l(k', k; E) = V_l(k', k) + \frac{2}{\pi} \int_0^\infty dq q^2 \frac{V_l(k', q) T_l(q, k; E)}{E - E_q + i\epsilon}, \quad (56)$$

with $E_q \equiv q^2/m$. Note that this equation can be solved for any values of k' , k , and E . But if we want to relate T_l to the scattering amplitude $f_l(k)$, we have to evaluate it *on shell*:

$$T_l(k, k; E = E_k) = -\frac{2\pi}{\mu} f_l(k), \quad (57)$$

meaning that $k' = k$ and the energy is $k^2/2\mu$. However, to solve the LS equation (56) for on-shell conditions on the left side, we need $T_l(q, k; E_k)$ in the integral. So $q \neq k$ and we call this “half-on-shell”. We will talk more about “on-shell” and “off-shell”; for now we just remark that it is impossible to make an absolute determination of off-shell behavior (despite past attempts to design nuclear experiments to do exactly that!).

If we keep only the first term, then $T = V$ and this is the Born approximation. If we approximate T on the right side by V , this is the second Born approximation. We can keep feeding the approximations back (i.e., we iterate the equation) to generate the *Born series*. It is analogous to the familiar perturbation theory from quantum mechanics. In operator form, the Lippman-Schwinger equation and the Born series expansion is

$$\widehat{T}(z) = \widehat{V} + \widehat{V} \frac{1}{z - \widehat{H}_0} \widehat{T}(z) = \widehat{V} + \widehat{V} \frac{1}{z - \widehat{H}_0} \widehat{V} + \widehat{V} \frac{1}{z - \widehat{H}_0} \widehat{V} \frac{1}{z - \widehat{H}_0} \widehat{V} + \dots \quad (58)$$

Check that taking matrix elements between momentum states and evaluating at $z = E + i\epsilon$ reproduces our previous expressions Eqs. (55) and (56). [*Exercise!*]

Note that the difference between a local and a non-local potential is not noticeable at the level of the partial wave LS equation. But still, given the freedom, why *not* choose local? You’ll find an argument in favor of non-local potentials when we consider the NN interaction and what a local form implies about short-range repulsion. A special type of non-local potential is a *separable* potential:

$$\widehat{V} = g|\eta\rangle\langle\eta|, \quad (59)$$

where g is a constant. Then $V_l(k', k) = g\eta(k')\eta(k)$ where $\eta(k) = \langle k|\eta\rangle$, and similarly in (partial-wave) coordinate space. It is straightforward to show (don’t you hate it when people say that? :) that $\widehat{T}(z)$ in Eq. (58) is also separable and the Lippman-Schwinger equation can be solved *algebraically*.

e.2 Computational methods for phase shifts: Matrix solution of Lippmann-Schwinger equation

To solve the LS equation numerically, we generally turn to a different function that satisfies the same equation but with a principal value rather than $+i\epsilon$. Landau in his QMII book calls this the

R-matrix but it is also called the K-matrix elsewhere. In the exercises we work out the numerical evaluation of the R-matrix to calculate phase shifts.

The plan whenever possible for computational effectiveness is to use matrix operations (e.g., multiply two matrices or a matrix times a vector), which are efficiently implemented. The partial wave Lippmann-Schwinger equation is an integral equation in momentum space that, with a finite *discretization* of the continuous range of momentum in a given partial wave, naturally takes the form of matrix multiplication.

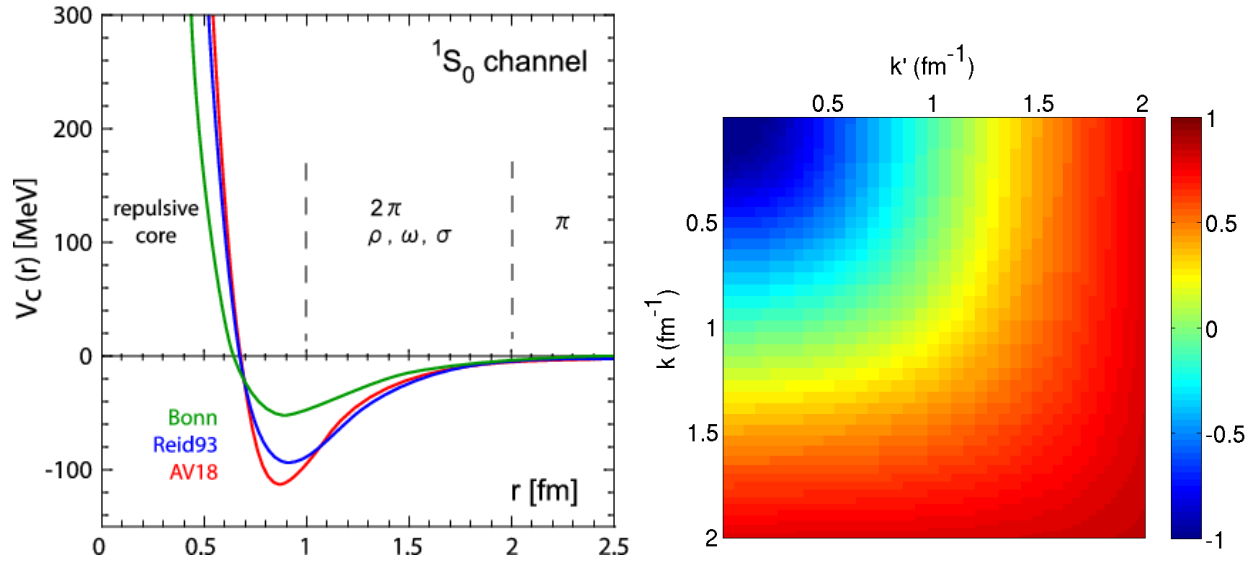


Figure 4: On the right is a matrix version of the 1S_0 AV18 potential on the left.

$$V_{L=0}(k, k') \propto \langle k | V_{L=0} | k' \rangle \propto \int d^3r j_0(kr) V(r) j_0(k'r) \implies V_{kk'} \text{ matrix} . \quad (60)$$

Two-minute question: What would the kinetic energy look like on the right figure of Fig. 4? To set the scale on the right in Fig. 4, recall our momentum units ($\hbar = c = 1$). The typical relative momentum in a large nucleus is $\approx 1 \text{ fm}^{-1} \approx 200 \text{ MeV}$.

f. Effective range expansion

As first shown by Schwinger, $k^{2l+1} \cot \delta_l(k)$ has a power series expansion in k^2 (see Newton for more details on proving this). The radius of convergence is dictated by how the potential falls off for large r ; for a Yukawa potential of mass m , this radius is $m/2$. For $l = 0$ the expansion is

$$k \cot \delta_0(k) = -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 - P r_0^3 k^4 + \dots , \quad (61)$$

which defines the S -wave *scattering length* a_0 , the S -wave *effective range* r_0 and the S -wave *shape parameter* P (often these are written a_s and r_s or a and r_e). Note the sign conventions. For $l = 1$

the convention is to write

$$k^3 \cot \delta_1(k) = -\frac{3}{a_p^3}, \quad (62)$$

which defines the P -wave scattering length a_p (with dimensions of a length).

The effective range expansion for hard-sphere scattering (radius R) is (just do the Taylor expansion with $\delta_0(k) = -kR$):

$$k \cot(-kR) = -\frac{1}{R} + \frac{1}{3}Rk^2 + \dots \implies a_0 = R \quad r_0 = 2R/3 \quad (63)$$

(note the sign of a_0) so the magnitudes of the effective range parameters are all the order the range of the interaction R . The radius of convergence here is infinite because the potential is identically zero beyond some radius.

For more general cases, we find that while $r_0 \sim R$, the range of the potential, a_0 can be anything:

- if $a_0 \sim R$, it is called “natural”;
- $|a_0| \gg R$ (unnatural) is particularly interesting, e.g., for neutrons or cold atoms.

We can associate the sign and size of a_0 with the behavior of the scattering wave function as the energy (or k) goes to zero, since

$$\frac{\sin(kr + \delta_0(k))}{k} \xrightarrow{k \rightarrow 0} r - a_0, \quad (64)$$

so in the asymptotic region the wave function is a straight line with intercept a_0 (see Fig. 5). We see that a_0 ranges from $-\infty$ to $+\infty$ (are there excluded regions?).

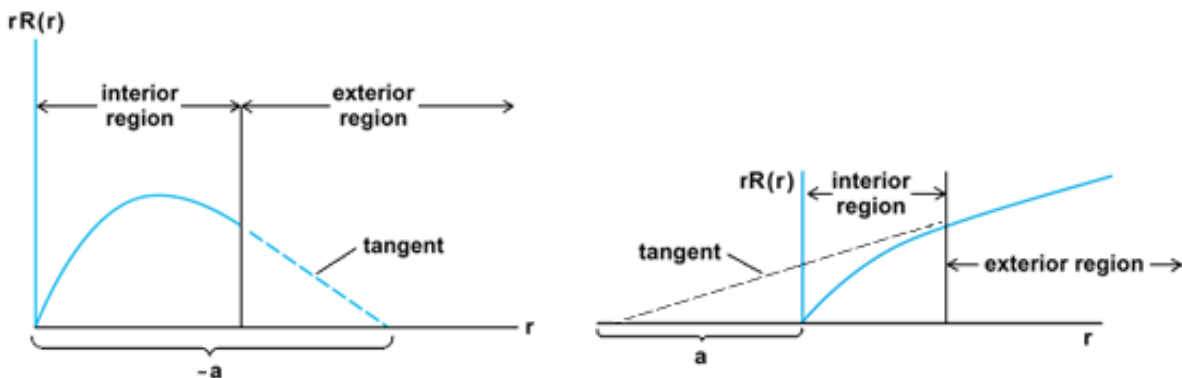


Figure 5: Identifying the S -wave scattering length a_0 by looking at $k \rightarrow 0$ wave functions. [credit to ???]

Let us consider the case of low-energy scattering for $l = 0$. Then the S -wave scattering amplitude is (recall Eq. (20))

$$f_0(k) = \frac{1}{-1/a_0 - ik} \implies \sigma(k) = \frac{4\pi}{1/a_0^2 + k^2}. \quad (65)$$

In the natural case, $|ka_0| \ll 1$ and $f_0(k) \rightarrow -a_0$ at low k and

$$\frac{d\sigma}{d\Omega} = a_0^2 \quad \implies \quad \sigma = 4\pi a_0^2. \quad (66)$$

Also, $\delta_0(k) \approx -ka_0$ implies that the sign of a corresponds to the sign of V (if strictly attractive or repulsive). Figure 5 tells us that to get large a_0 (unnatural), we need to have close to a zero-energy bound state (so the wave function is close to horizontal in the asymptotic region). If $a_0 > 0$, we have a shallow bound state (i.e., close to zero binding energy) while if $a_0 < 0$ we have a nearly bound (virtual) state. The limit of $|a_0| \rightarrow \infty$ is called the unitary limit; the cross section becomes

$$\frac{d\sigma}{d\Omega} \rightarrow \frac{1}{k^2} \quad \implies \quad \sigma = \frac{4\pi}{k^2}, \quad (67)$$

which is the largest it can be consistent with the constraint of unitarity.

We can associate the observations about bound or near-bound states for large a_0 with the analytic structure of $f_0(k)$ continued to the complex k plane. Poles on the positive real axis correspond to bound states while those on the negative real axis to virtual bound states. From Eq. (65), for $a_0 > 0$ the pole is at $k = i/a_0$, so we have a bound-state as advertised, with a pole in energy at the bound state value: $E \approx -\hbar^2|k|^2/2\mu = -\hbar^2/(2\mu a_0^2)$. [Check!] (You'll see how this analytic structure plays out for a square well in the exercises.) We get a better estimate of the bound-state energy by keeping the effective range term as well in $f_0(k)$.

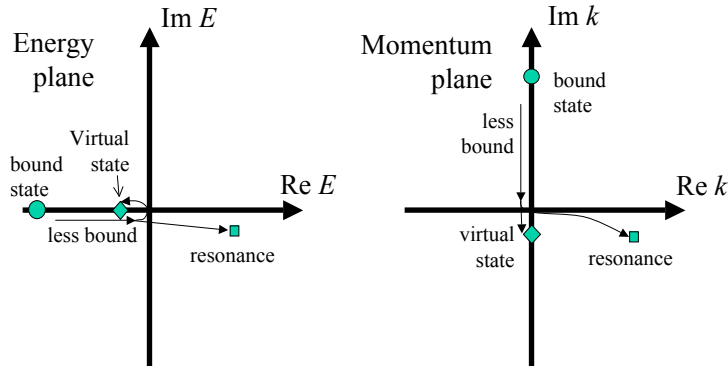


Figure 6: From Filomena Nunes notes: “The correspondences between the energy (left) and momentum (right) complex planes. The arrows show the trajectory of a bound state caused by a progressively weaker potential: it becomes a resonance for $L > 0$ or when there is a Coulomb barrier, otherwise it becomes a virtual state. Because $E \propto k^2$, bound states on the positive imaginary k axis and virtual states on the negative imaginary axis both map onto the negative energy axis.” [See K.W. McVoy, Nucl. Phys. A, **115**, 481 (1968) for a discussion of the difference between virtual and resonance states.]

Schwinger first derived the effective range expansion (ERE) back in the 1940’s and then Bethe showed an easy way to derive (and understand) it. This is apparently a common pattern with Schwinger’s work! The implicit assumption here is that the potential is short-ranged; that is, it falls off sufficiently rapidly with distance. This is certainly satisfied by any potential that actually

vanishes beyond a certain distance. Long-range potentials like the Coulomb potential must be treated differently (but a Yukawa potential, which has a finite range although non-vanishing out to $r \rightarrow \infty$, is ok).

When first identified, the ERE was a disappointment because it meant that scattering experiments at low energy could not reveal the structure of the potential. For example, it is impossible to invert the expansion at any finite order to find a potential that correctly gives scattering at higher energies. All you determined were a couple of numbers (scattering length and effective range) and any potential whose ERE was fit to these would reproduce experimental cross sections. In the modern view we are delighted with this: the low-energy theory is determined by a small number of constants that encapsulate the limited high-energy features that affect the low-energy physics (in many ways like a multipole expansion; see exercises for later lectures). We can devise an effective theory (called the “pionless effective theory”) to reproduce the ERE and consistently extend it to include the coupling to external probes (and other physics).