Scattering Tutorial

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This tutorial is derived from an appendix to my thesis (`http://www.physics.ohio-state.edu/~emueller/thesis`). It covers the standard physics of low-energy s-wave scattering as found in textbooks [1]. It attempts to be pedagogical. See `http://www.physics.ohio-state.edu/~emueller/scatter` for supplementary Java programs.

1 The Scattering amplitude

1.1 Definition

The basic picture of potential scattering is illustrated in Fig. 1. One has an incoming wave e^{ikz} that is incident on a small impurity of size r_0 (positioned at the origin), and one asks what the far field wavefunction looks like. Generically

$$\psi(r) = e^{ikz} + f(k, \hat{r})\frac{e^{ikr}}{r}, \qquad (1)$$

which has the form of the incoming wave plus a scattered wave. In the far field $r \gg r_0$, the scattering amplitude f can only be a function of the incident wave vector k, and on the direction $\hat{r}$. (In this equation f is also implicitly a function of the direction of the incoming wave, generically denoted $\hat{k}$ and here set to $\hat{z}$. For a spherically symmetric potential f is independent of $\hat{k}$.)

In the long wavelength limit $kr_0 \ll 1$ one expects that the scattering will become isotropic – the wave is too large to "see" the structure of the impurity. Thus one can drop the $\hat{r}$ dependences and only consider $f(k)$, referred to as the s-wave scattering amplitude. All of our discussions will be limited to this s-wave limit. The same argument implies that f does not have much momentum dependence. For the most part this statement is true and f can be replaced by $f(k = 0)$; however in the presence of a scattering resonance, f depends strongly on k. These resonances are of immense experimental importance.

It is worth mentioning that resonant scattering in higher momentum channels ("shape resonances"), can lead to angular dependence of f in the long wavelength limit. These resonances play no roles in current alkali gas experiments.
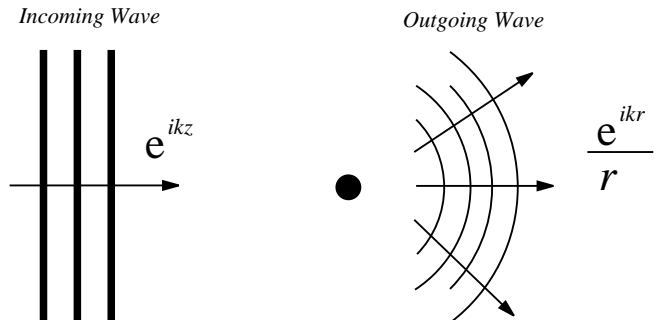
Figure 1: Generic Scattering Geometry. An incoming plane wave e^{ikz} reflects off a small impurity.

1.2 T-matrix

There are two problems in scattering theory. First, relating the scattering amplitude to the scattering potential, and second, relating the properties of the system to the scattering amplitude. The first problem amounts to solving the Schrödinger equation in the presence of the impurity, with the boundary condition that the incoming wave is e^{ikz}. Generically solving this equation requires the use of computers, but in principle is solvable to arbitrary precision.

As an alternative to computers, one can also use perturbation theory to solve the Schrödinger equation. For realistic atomic potentials perturbation theory is not going to work well. Nevertheless it is still useful to formally develop the scattering amplitude as a sum of terms, each one containing higher powers of V. One can then think of the scattered wavefunction as coming from multiple scattering from the impurity.

The standard approach to developing the perturbation series is to write the Schrödinger equation in integral form. Formally I write

$$\psi = \phi - \frac{1}{H_0 - E} V \psi, \tag{2}$$

where $\phi = e^{ikz}$ is the incident wave function, V is the scattering potential, $E = k^2/2m$ is the energy of the state, and $(H - E)^{-1}$ is the Green's function for the free Schrödinger equation. Applying $H_0 - E$ to Eq. (2), one arrives at

$$(H_0 - E)\psi = -V\psi, \tag{3}$$

which is the conventional Schrödinger equation.

As can be verified directly, in momentum space and in real space, the Green's functions are given by

$$\langle q| \frac{1}{H - E} |q'\rangle \;\; = \;\; \frac{(2\pi)^3 \delta^3(q - q')}{q^2/2m - E} \tag{4}$$

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$$\langle r|\frac{1}{H-E}|r'\rangle \quad = \quad \frac{m}{2\pi}\frac{\exp(ik|r-r'|)}{|r-r'|}, \tag{5}$$

where $E = k^2/2m$. On physical grounds, I have chosen outgoing boundary conditions in Eq. (5). This latter result is only true in three dimensions. Getting away from my schematic notation, one writes Eq. (2) in one of two forms,

$$\psi(\mathbf{k}') \quad = \quad (2\pi)^3\delta^3(k\hat{\mathbf{z}}-\mathbf{k}') - 2m\int\frac{d^3q}{(2\pi)^2}\frac{V(k'-q)}{q^2-(k')^2}\psi(\mathbf{q}), \tag{6}$$

$$\psi(\mathbf{r}) \quad = \quad e^{ikz} - \frac{m}{2\pi}\int d^3r'\,\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(r')\psi(r'), \tag{7}$$

The first equation is in momentum space, the second in real space. In this Section I only consider the real space equation (7), though later I will focus on (6). For simplicity I assume that $V(r)$ falls off over a lengthscale r_0. Longer range potentials can be treated, but such analysis is not particularly important for discussing neutral atoms.

In the far field, $r \gg r_0$, one can expand the difference $|\mathbf{r}-\mathbf{r}'|$ in the integral, to arrive at the equation

$$\psi(r) = e^{ikz} - \frac{m}{2\pi}\frac{e^{ikr}}{r}\int d^3r'\,e^{ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(r')\psi(r'). \tag{8}$$

Comparison with Eq. (1) gives an expression for the scattering amplitude,

$$f(k,\hat{r}) = -\frac{m}{2\pi}\int d^3r'\,e^{ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(r')\psi(r'). \tag{9}$$

One generates a perturbative solution to Eq. (7) by a simple iterative scheme. One starts by setting $\psi(r) = e^{ikz}$ on the right hand side of (7). This first order result is known as the Born approximation to scattering. This procedure is iterated by substituting the new value of ψ into the right hand side. In a schematic notation, one has

$$\psi = \left(1 - \frac{1}{H_0-E}V + \frac{1}{H_0-E}V\frac{1}{H_0-E}V + \frac{1}{H_0-E}V\frac{1}{H_0-E}V\frac{1}{H_0-E}V + \cdots\right)\phi. \tag{10}$$

This expression is compactly written as

$$\psi = \psi_0 - \frac{1}{H_0-E}T\psi_0, \tag{11}$$

where the T-matrix is defined by

$$T \quad = \quad V + V\frac{1}{H_0-E}V + V\frac{1}{H_0-E}V\frac{1}{H_0-E}V + \cdots \tag{12}$$
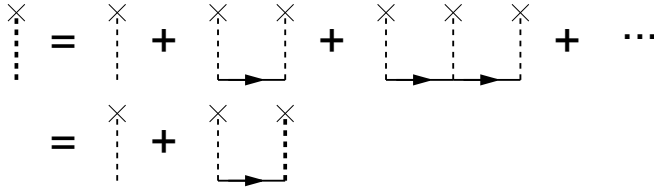
$$= \quad V + V\frac{1}{H_0-E}T. \tag{13}$$

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Figure 2: Diagrammatic representation of the T-matrix equation. The T-matrix, designated by a dark dashed line connected to an "X", comes from multiple scattering off the potential. The soft dashed lines represent bare potential scattering.

A diagrammatic representation of Eq. (12) is shown in Fig. 2. The scattering amplitude is then related to the on-shell T-matrix, by the expression

$$f(k) = \frac{-m}{2\pi\hbar^2} T(k). \tag{14}$$

For the many-body problem, or for the problem of scattering off many impurities, one in principle needs the off shell T-matrix.

To fully appreciate the structure of the T-matrix, one must go beyond s-wave scattering, and consider the generic scattering amplitude $f(\hat{k}, \hat{r}, k)$ defined by the asymptotic form

$$\psi(r) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(k, \hat{k}, \hat{r})\frac{e^{ikr}}{r}. \tag{15}$$

The scattering amplitude is a function of the direction of the incoming wave $\hat{k}$, the direction of the outgoing wave $\hat{r}$, and the energy of the scattering particle, $k^2/2m$.

The T-matrix similarly is a function of three variables,

$$T(\mathbf{k}, \mathbf{k}', q) \equiv \langle k'|T(E = q^2/2m)|k\rangle \tag{16}$$

$$= \langle k'|V|k\rangle + \langle k'|V\frac{1}{H_0 - E}T|k\rangle. \tag{17}$$

The variables are the incoming momentum $\mathbf{k}$, the outgoing momentum $\mathbf{k}'$, and the energy $E = q^2/2m$. If one sets $|k| = |k'| = q$, one finds

$$f(k, \hat{k}, \hat{r}) = -\frac{m}{2\pi}T(k\hat{k}, k\hat{r}, k). \tag{18}$$

The off mass shell terms of T give information about the non-asymptotic behavior of the scattering. If one throws away all this information, such as one does in the pseudo-potential approximation, one finds that the T-matrix is independent of the momenta $\mathbf{k}$ and $\mathbf{k}'$, and is only a function of the energy q

$$T(\mathbf{k}, \mathbf{k}', q) = T(q) = \frac{-2\pi}{m}f(q). \tag{19}$$

This approximation will clearly break down when the momenta are of atomic dimensions.

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1.3 Phase shifts

In the limit of s-wave scattering, the impurity only sees the part of the incoming wave that is spherically symmetric. One finds the spherically symmetric part of the incoming wave by integrating over the solid angle,

$$\int \frac{d\Omega}{4\pi} e^{ikz} = \frac{1}{2} \int_{-1}^{1} d\cos\theta \, e^{ikr\cos\theta} \tag{20}$$

$$= \frac{\sin(kr)}{kr}. \tag{21}$$

This wave has components which are propagating towards and away from the impurity, as is seen by representing the wavefunction as

$$\frac{\sin(kr)}{kr} = \frac{-1}{2i} \frac{e^{-ikr}}{kr} + \frac{1}{2i} \frac{e^{ikr}}{kr}. \tag{22}$$

The scattering can only affect the outgoing wave. Since particles are conserved, the only possible change it can make to the outgoing wave (in the asymptotic region) is to provide a phase shift, δ,

$$e^{ikr} \rightarrow e^{i(kr+2\delta)} = e^{ikr} + 2ie^{ikr}e^{i\delta}\sin\delta. \tag{23}$$

Thus, in complete generality, one can write the scattered wavefunction as

$$\psi(r) = e^{ikz} + \frac{e^{i\delta}\sin\delta}{k} \frac{e^{ikr}}{r}. \tag{24}$$

Comparing with Eq. (1) one arrives at an expression for the scattering amplitude in terms of the phase shift.

$$f(k) = e^{i\delta}\sin\delta/k. \tag{25}$$

1.4 Meaning of the scattering amplitude and the phase shift

On a microscopic level, δ has a clear meaning. It is the phase shift of the scattered wave, relative to what it would be without the impurity. In the following section I will show how this phase shift can be simply related to the density of states in the presence of the impurity. The scattering amplitude, f, is the amplitude that the particles are scattered. That is, $\sigma = 4\pi|f|^2$ is the number of scattered particles per unit flux of incoming particles. The cross section σ is the area that a classical target would have to have for the scattering probability to be the same.

An equivalent way to understand f is to look at the equation

$$\psi = e^{ikz} + f\frac{e^{ikr}}{r}. \tag{26}$$

The length f gives the distance from the impurity at which the flux of scattered particles equals the flux of incoming particles.

For small δ Eq. (25) can be expanded, and one finds that $f \approx \delta/k$.

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2 Relationship of the scattering problem with the standing wave problem

In elementary quantum mechanics, the first problem one learns to solve is the "particle in a box." One takes the Hamiltonian $-\hbar^2\nabla^2/2m$, diagonalizes it via a Fourier series, and finds the complete spectrum. Later one learns how to do scattering problems, where one is not interested in the spectrum (which is continuous), but rather on transmission and reflection amplitudes. The relationship between these two problems is rarely completely clear.

One can connect the scattering problem and the standing wave problem by looking at scattering in a finite size box. The three dimensional case (when limited to the s-wave channel) is actually simpler than the one dimensional problem, so I will concentrate on it. I first "solve" the standing wave problem. Consider a small impurity with a potential $V(r)$ in the middle of a big spherical box of radius R. I wish to find the eigenvalues of the Schrödinger equation,

$$\left[\frac{-\nabla^2}{2m} + V(r) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{27}$$

with the boundary condition that $\psi(R) = 0$. I take $\hbar = 1$, and restrict myself to spherically symmetric states. By substituting $\psi(r) = u(r)/r$, one can write s-wave sector of the Schrödinger equation as

$$\left[\frac{-1}{2m} \frac{d^2}{dr^2} + V(r) \right] u(r) = Eu(r), \tag{28}$$

with the boundary condition $u(0) = u(R) = 0$. For r larger than the range of the potential, one can ignore $V(r)$, and this equation is just a free one dimensional Schrödinger equation. Thus in the asymptotic regime there is some δ such that the solution to (28) is $u(r) = \sin(kr + \delta)$. To satisfy the boundary conditions the momentum k must obey $kR + \delta = n\pi$, for some integer n.

Now imagine one performs a scattering experiment on the same potential. One sends in a wave $u(r) \sim e^{-ikr}$, and looks at what comes out. Thus one must solve Eq. (28) with the condition that the incoming part of u is $(-1/2i)e^{-ikr}$. Well, we know one solution of Eq. (28), which asymptotically is $u(r) = \sin(kr + \delta)$. Multiplying by $-2ie^{i\delta}$, one gets $u(r) = e^{-ikr} - e^{ikr}e^{2i\delta}$. Since solutions to the Schrödinger equation with a given boundary condition are unique, this u must be the scattered wavefunction. Comparing with Eq. (23), one sees that the δ which arises in solving the standing wave problem is the same as the δ which appears in the scattering problem. With this relationship one can solve the scattering problem by using the powerful computational techniques which have been developed for ground-state problems (see for example [2]).

2.1 Energy shifts

The relationship between scattered states and standing waves gives rise to a very nice graphical construction which allows one to relate the density of states
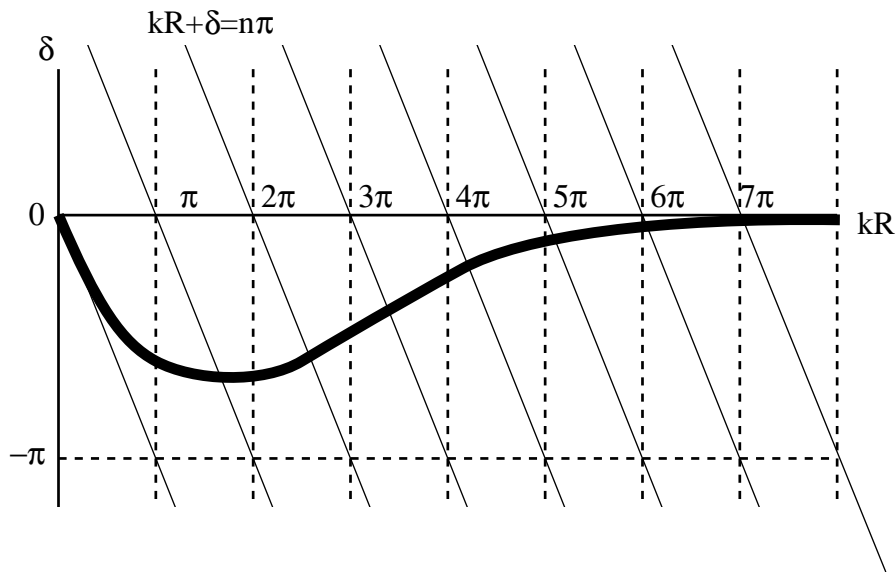
Figure 3: Connecting phase shifts and energy shifts. The thick line represents the phase shift $\delta(k)$. In a box, $\sin(kR + \delta) = 0$, so the allowed states lie at the intersection of the thick line and the oblique lines $kR + \delta = 0$. As the box is made larger, the spacing between the oblique lines becomes smaller, and (on an absolute scale) they become more perpendicular to the k axis.

to the phase shifts. Imagine one knows the phase shifts $\delta(k)$ (for example, see Fig. 3). If one places the system in a box, the only states which obey the boundary conditions have $kR + \delta = n\pi$ for some integer n. Thus the allowed states have a wave vector given by the intersection of the lines $kR + \delta = n\pi$ and $\delta(k)$.

In the absence of an impurity the wave vectors allowed have $kR = n\pi$. Thus the shift in wave vector is $\delta k = -\delta/R$, and the change in the energy of a state is $\delta E = k\,\delta k/m = -\delta\,k/mR$, which is proportional to δ. As a historical note, this result was a point of confusion in the 1950's in the context of the many-body problem [3].

In the limit of large box, it is more convenient to talk about a density of states, rather than the energy of any particular state. Starting from the relation $kR + \delta = n\pi$, one finds that the density of s-wave states in k-space is

$$\frac{\partial n}{\partial k} = \frac{R}{\pi} + \frac{\delta'(k)}{\pi}, \tag{29}$$

where $\delta'(k)$ is the derivative of δ with respect to k. The first term is the standard density of states in a 1-dimensional box, while the second term is the change in the density of states due to the impurity. Thus one interprets δ/π as the number of extra states with momentum less than k due to the impurity.

If one knows the density of states, then one can calculate For example, consider a spherical "bump" potential as depicted in Fig. 4. The bump has
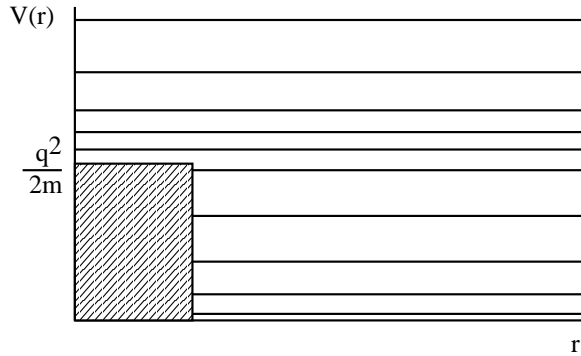
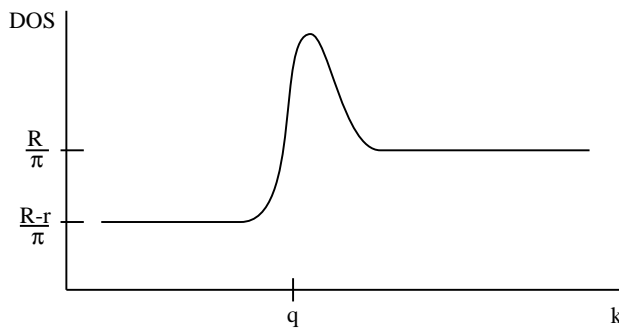Figure 4: Energy states for a spherical bump in a box. States are pushed up by the bump

Figure 5: Density of states for a spherical bump in a box (schematic). The potential has a height of $V_0 = q^2/2m$, and width r.

radius r_0 and height $q^2/2m$. For $k \ll q$, the bump appears to be an infinite barrier, and the density of states should be $\partial n = (R - r_0)/\pi\,\partial k$, which is less than the density of states in the absence of the bump. The missing states have to go somewhere, and they are pushed to momenta near $k = q$. For $k \gg q$, the bump is irrelevant, and the density of states should be that of a free gas, $\partial n = R/\pi\,\partial k$. One should therefore see a density of states like the one in Fig. 5. After integrating this curve, one arrives at a phase shift δ like the one depicted in Fig. 6.

As a corollary to the theorem that $\delta(k)/\pi$ is the number of extra states, one has the general result that for a sufficiently well-behaved potential the $k = 0$ the phase shift is equal to π times the number of bound states. Generically $\delta(k \to \infty) = 0$, and the bound states are missing from the continuum.
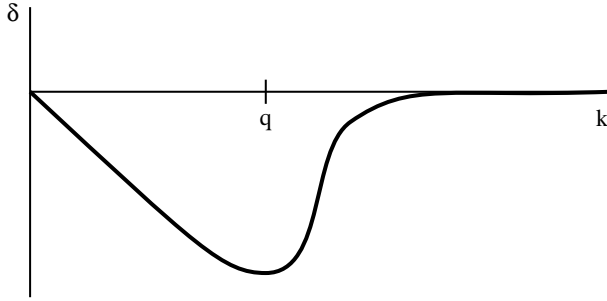
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Figure 6: Phase shift for a spherical bump in a box (schematic). The height of the potential is $q^2/2m$.

3 Sample phase shifts

In this section I plot a few illustrative phase shifts.

3.1 Hard wall

The simplest scattering potential is a hard wall:

$$V(r) = \begin{cases} \infty & r < r_0 \\ 0 & r > r_0. \end{cases} \tag{30}$$

The wavefunction must vanish at the edge of the wall, so $u(r) = \sin(k(r - r_0))$ and $\delta = -kr_0$. This example is pathological in that $\delta \to \infty$ as $k \to \infty$.

3.2 Attractive well

A slightly more complicated simple potential is the attractive spherical well,

$$V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0. \end{cases} \tag{31}$$

This potential is not realistic but it possesses many of the features of more sophisticated atomic potentials. In particular there are low energy resonances whenever a new bound state enters the well. To find the phase shifts I write the wavefunction as

$$u(r) = \begin{cases} A\sin(k'r) & r < r_0 \\ B\sin(kr + \delta) & r > r_0, \end{cases} \tag{32}$$

where $(k')^2/2m - V_0 = k^2/2m$. Continuity of the wavefunction and its derivative are guaranteed by matching the logarithmic derivative at r_0, which gives

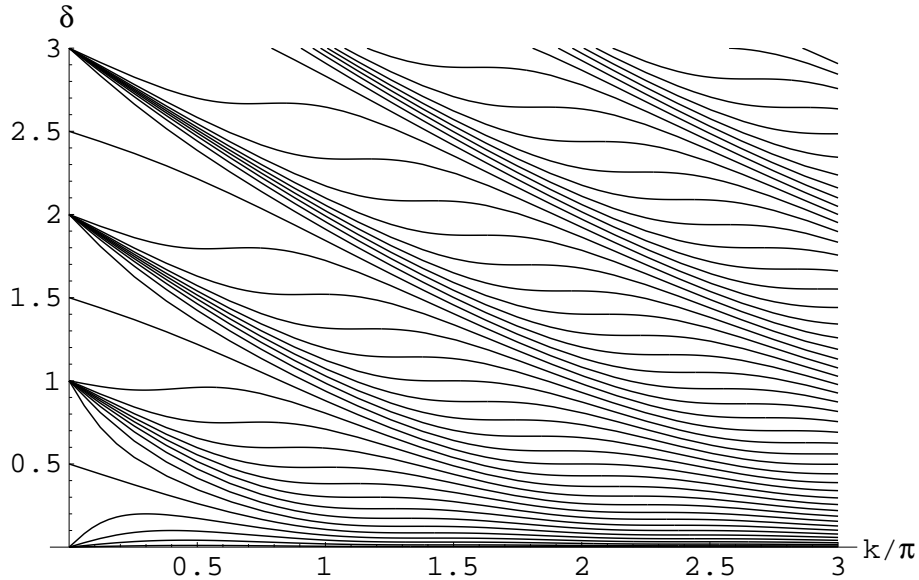$$k'\cot(k'r_0) = k\cot(kr_0 + \delta). \tag{33}$$

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Figure 7: Phase shifts for a spherical well potential. The depth of the well is $V_0 = q^2/2m$ and its radius is r_0. All momenta are measured in terms of r_0. The various lines show different values of q, each differing by $0.1\pi/r_0$. Resonances occur at $qr_0 = (n + 1/2)\pi$.

Solving for δ gives

$$\tan \delta = \frac{k \sin k'r_0 \cos kr_0 - k' \sin kr_0 \cos k'r_0}{k' \cos k'r_0 \cos kr_0 + k \sin kr_0 \sin k'r_0}. \tag{34}$$

For different values of V_0 I plot $\delta(k)$ in Fig. 7. For simplicity I introduce the momentum q, satisfying $V_0 = q^2/2m$, which marks the depth of the well. The most striking feature of these graphs is that when $\cos(qr_0) = 0$, the phase shift at $k = 0$ jumps. This happens because a new bound state enters the well at this point.

It is instructive to put this system in a box of size R, and calculate the energy of the first few levels as a function of q. As seen in Fig. 8, whenever one passes through a resonance, the lowest energy state becomes bound, and the next level replaces it. What is happening is that each line has a fixed number of nodes, and at the resonance one of the nodes moves from outside the well to inside the well, drastically reducing the energy.
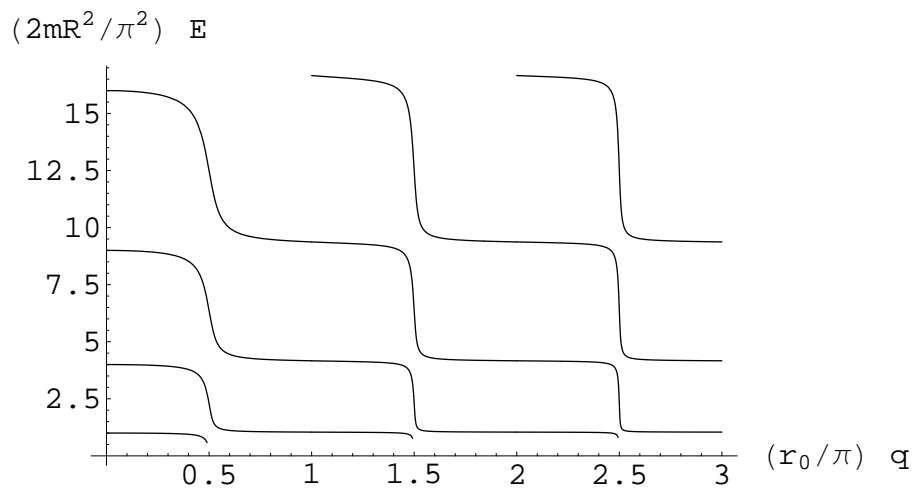
$(2mR^2/\pi^2)$ E

15

12.5

10

7.5

5

2.5

0.5   1   1.5   2   2.5   3 (r_0/π) q

Figure 8: Energy levels for an attractive well of radius r_0 and depth $V_0 = q^2/2m$ within a box of size R. The energy is measured in terms of the quantization energy of the large box, π^2/mR^2. The horizontal axis shows qr_0/π, a measure of the depth of the well. Resonances occur whenever $qr_0 = (n + 1/2)\pi$, and one of the continuum energy states drops into the well. For this plot $R = 50r_0$. Increasing R_0 makes the jumps sharper.
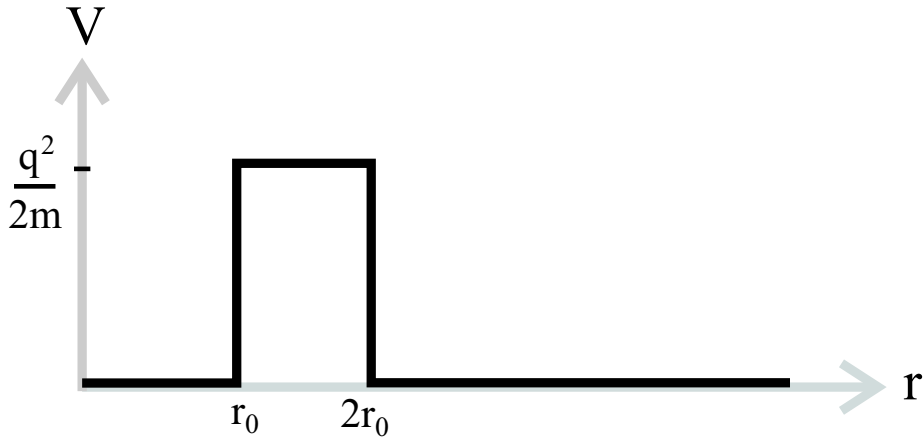
Figure 9: Resonant barrier potential.

3.3 Resonant barrier

I next consider a resonant barrier potential, as shown in Fig. 9,

$$
V(r) = \begin{cases} 0 & r < r_0 \\ q^2/2m & r_0 < r < 2r_0 \\ 0 & r > 2r_0. \end{cases} \tag{35}
$$

As opposed to the attractive well which possesses zero energy resonances, the resonant barrier has finite energy resonances resulting from the quasi-bound states which are found at momenta where $\sin(kr_0) \approx 0$. At these resonances, one finds an extra state. From our understanding of δ'/π as the density of states, we should have a phase change of π near this momentum. As seen in Fig. 10, this is indeed the case.

4 The pseudopotential

Here I discuss an expansion of the scattering amplitude in powers of kr_0, where r_0 is the length scale of the potential. This expansion takes the form

$$
k \cot \delta = -\frac{1}{a_s} + \frac{1}{2} r_e k^2 + \mathcal{O}((r_0 k)^4). \tag{36}
$$

The parameters a_s and r_e are known as the scattering length and the effective range. I emphasize that (36) is an expansion in $r_0 k$, and even when a_s is large, the remaining terms can be small. The pseudopotential approximation amounts to taking only the first term in this expansion.

One derives Eq. (36) via a matching argument. The Schrödinger equation obeyed by $u(r) = r\psi(r)$ is

$$
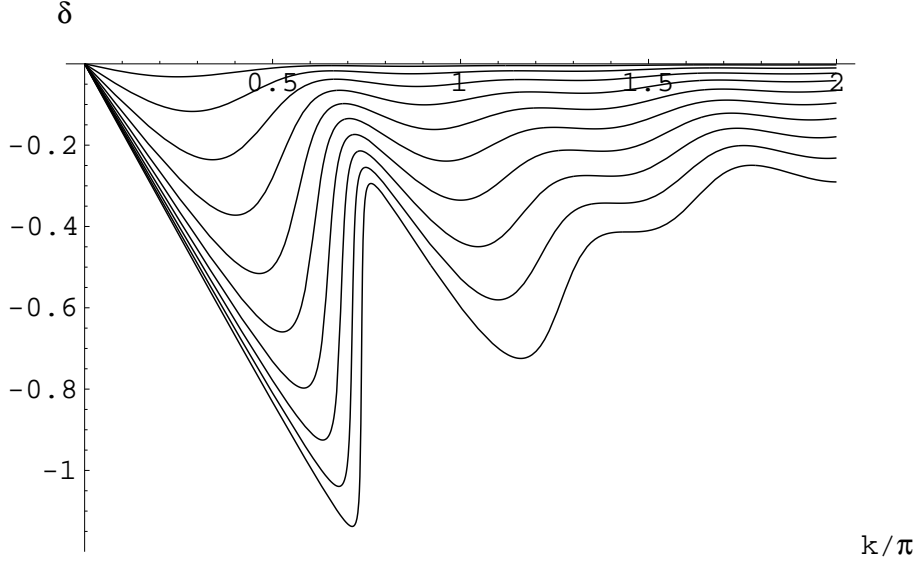\left(\frac{k^2 + \partial_r^2}{2m} - V(r) \right) u = 0. \tag{37}
$$

Figure 10: Phase Shifts $\delta(k)/\pi$ for a resonant barrier potential. The momentum k is measured in units of π/r_0. Each line corresponds to a different barrier height.

For $r \ll r_0$, $V(r)$ dominates over k^2, and one writes

$$u(r) = \chi(r) + \mathcal{O}(k^2), \qquad r \ll r_0, \tag{38}$$

where $\chi(r)$ is independent of k. For $r \gg r_0$, the potential $V(r)$ vanishes and u takes on its asymptotic form

$$u(r) = A \sin(kr + \delta), \qquad r \gg r_0. \tag{39}$$

I match the logarithmic derivatives at r_0, finding

$$k \cot(kr_0 + \delta) = \chi'/\chi + \mathcal{O}(k^2), \tag{40}$$

which gives the desired expansion of $k \cot \delta$ in powers of k^2.

In terms of $\cot \delta$ the scattering amplitude is

$$f = \frac{e^{i\delta} \sin \delta}{k} = \frac{1}{k \cot \delta + ik}. \tag{41}$$

So in the pseudo-potential approximation, the scattering amplitude is

$$f = \frac{-a}{1 + ika}. \tag{42}$$

For small ak, this looks like a point interaction. For large values of ak, this looks like a long-ranged $1/k$ potential.
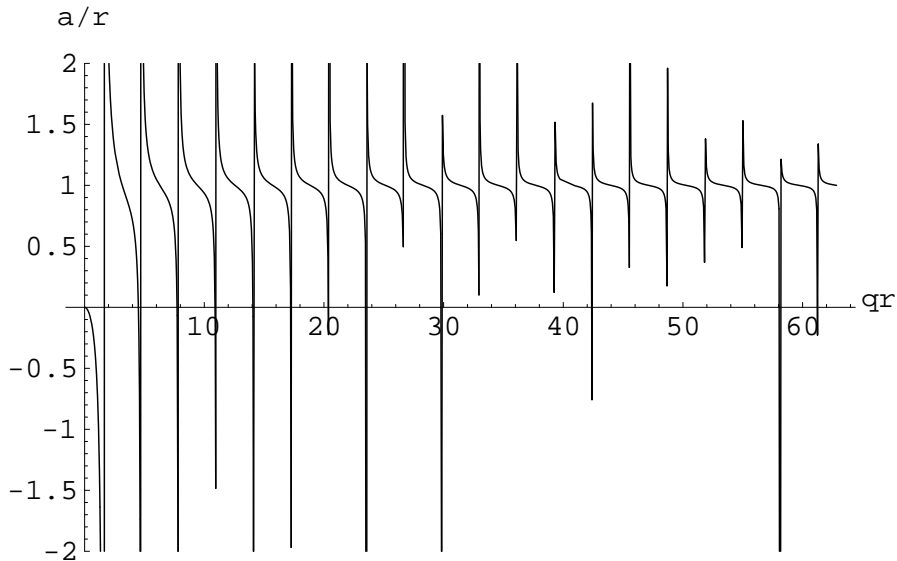
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Figure 11: Scattering length a for a spherical well of radius r and depth $V_0 = q^2/2m$.

4.1 The pseudo-potential for an attractive spherical well

As an example, one can expand Eq. (34) in powers of k, finding

$$k \cot \delta = \frac{-1}{a_s} + \frac{r_e k^2}{2} \tag{43}$$

$$a_s = r_0 - \frac{\tan q r_0}{q} \tag{44}$$

$$r_e = (\frac{1}{q} - r_0^2 q) \cos q r_o + r_0 \sin q r_0 + \frac{q^2 r_0^3 \cos^2 q r_0/3}{\sin q r_0 - q r_0 \cos q r_0}. \tag{45}$$

The effective range vanishes when a_s diverges. These quantities are plotted in Fig. 11 and 12.

5 Zero range potentials

For analytic calculations, the simplest potentials one can consider are zero-range potentials. These play an important role in many theoretical works, so it is worth considering them here. Zero range potentials are, by construction, singular. Thus, despite their analytic simplicity, these potentials require taking careful limits.
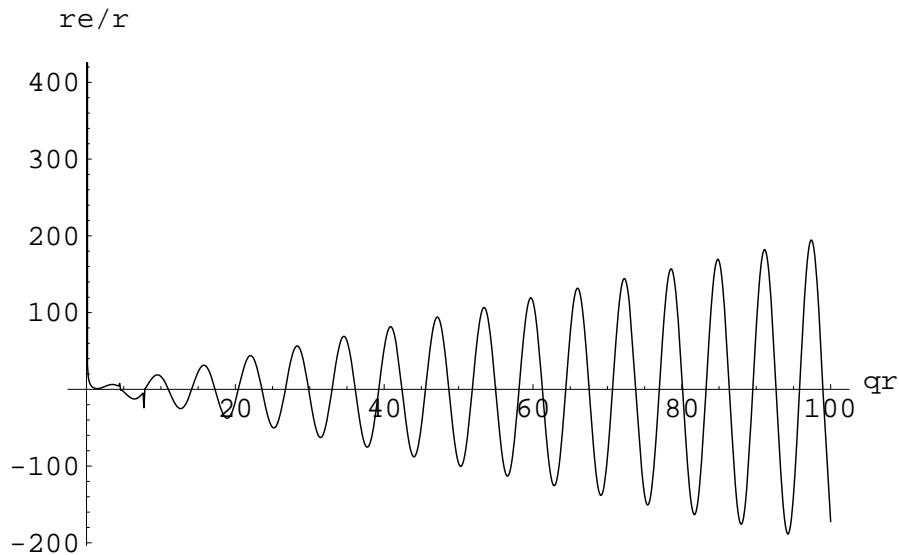
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Figure 12: Effective range re for a spherical well of radius r and depth $V_0 = q^2/2m$.

5.1 A structureless point scatterer

Consider a point scatterer with a potential $V(r) = V_0\delta(r - r')$. In momentum space, $V_k = V_0$. Scattering off this potential is described by the T-matrix equation (17),

$$T_{kk'}(\omega) = V_{kk'}(\omega + \sum_q V_{kq}G_0(q)T_{qk'}(\omega).$$ (46)

Since $V_{kk'}$ is independent of the momentum indices, T will also be independent of momentum. Using this result, the T-matrix is

$$T(\omega) = \frac{V_0}{1 - V_0\Theta},$$ (47)

where Θ is given by

$$\Theta = \sum_k G_0(q, \omega) = \sum_q \frac{1}{\omega - q^2/2m}.$$ (48)

Replacing the sum with an integral,

$$\Theta = \frac{V}{(2\pi)^3}\int \frac{d^3q}{\omega - q^2/2m}$$ (49)

$$= \frac{V}{2\pi^2}\int \frac{dq\, q^2}{\omega - q^2/2m},$$ (50)

15

one notices that the sum is ultraviolet divergent. This divergence is a consequence of the short range of the potential, and reflects the fact that a point interaction is unphysical. Any real potential will have a finite range, which will introduce a large q cutoff, Λ in this integral. The integral is readily evaluated to be

$$\Theta = \Theta_0 - \frac{imV\sqrt{2m\omega}}{2\pi} \tag{51}$$

$$\Theta_0 = -\frac{Vm\Lambda}{\pi^2}. \tag{52}$$

The T-matrix is then of the form

$$T = \frac{2\pi}{m} \frac{a_s}{1 + ia_s\sqrt{2m\omega}}, \tag{53}$$

where the scattering length is

$$a_s \equiv \frac{m}{2\pi} \frac{V_0}{1 - V_0\Theta_0}. \tag{54}$$

Note that if one takes the cutoff Λ to infinity at fixed V_0, then the scattering length vanishes. In this sense, there is no scattering off a delta-function potential in three dimensions. Only by scaling V_0 with Λ can a non-zero a_s be produced. This scaling of V_0 with Λ is the simplest example of *renormalization* which can be discussed. As previously discussed, a T-matrix of the form (53) gives a phase shift

$$\delta = \arg(T) = -\arctan(a_s k). \tag{55}$$

5.2 Scattering from a zero-range bound state

A simple generalization of the structureless point scatterer is to associate a bound state with the impurity. In such a case, the scattering is energy dependent, and

$$V_k = V_0 + \frac{|\alpha|^2}{\omega - \epsilon}, \tag{56}$$

where V_0 is a static potential at the origin, α is an amplitude for entering the bound state, and ϵ is the energy of the bound state. To illustrate the role of the bound state I set $V_0 = 0$, in which case

$$T = \frac{|\alpha|^2}{\omega - E + i(m/2\pi)|\alpha|^2\sqrt{2m\omega}}. \tag{57}$$

The energy E is

$$E = \epsilon + |\alpha|^2\Theta_0. \tag{58}$$

For E to be finite as $\Lambda \to \infty$ one must scale ϵ with Θ_0.

The T-matrix (57) leads to a phase shift of the form

$$\cot(\delta) = -\frac{1}{a_s k} + r_{\text{eff}}k^2/2, \tag{59}$$

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where

$$a_s = \frac{-m|\alpha|^2}{2\pi E} \tag{60}$$

$$r_{\text{eff}} = \frac{-2\pi}{m^2|\alpha|^2}. \tag{61}$$

A resonance occurs when $E = 0$.

The Green's function for the bound state is $T/|\alpha|^2$. Thus E *is* the energy of the bound. When $E > 0$, this state has a finite lifetime

$$\frac{1}{\tau} = \frac{m}{2\pi}|\alpha|^2\sqrt{2mE}, \tag{62}$$

which is the result one would expect from Fermi's golden rule.

6   Feshbach resonances

As is clear from the above examples, tuning a resonance near zero energy has dramatic consequences for atomic scattering properties. Experimentally such tuning is carried out by applying magnetic fields. The field induced resonance is known as a Feshbach resonance.

The underlying principle is that due to the hyperfine interaction, two colliding atoms can form a bound state whose magnetic moment is not equal to the sum of the magnetic moments of the incoming atoms (total angular momentum is conserved, not total magnetic moment). Consequently, when a magnetic field is applied, the Zeeman shift of the bound state can be different from the shift of the scattering states. Thus the energy of the bound state is tunable. When its energy is set to zero one is at the resonance. The scattering properties near the resonance are described well by the model of Section 5.2.

7   Multiple scattering

I now turn to the question of scattering off several small impurities which are much farther apart than the range of their potentials. As detailed in Section 4, low energy scattering off an individual impurity is described by the scattering length a_s. Letting n denote the density of scatterers, I am particularly interested in the limit where na_s^3 is of order 1. In this limit one encounters localization effects, and the scattering off of one impurity depends on the presence of all others.

7.1   Elementary approach

In this Section I frame the problem in terms of elementary quantum mechanics. Imagine that one has static impurities at positions $\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_n}$. The phase

shifts for scattering off any of these impurities is $\delta_0(k)$. In a scattering experiment, the asymptotic wavefunction will be

$$\psi(r) = e^{ikz} + \sum_i f_i \frac{e^{ik|r-r_i|}}{|r-r_i|}, \tag{63}$$

where the f_i's will be independent of space. This wavefunction should be good, except on atomic distances close to individual impurities. Comparing with Eq. (1), the scattering amplitude for scattering from the collection of impurities is

$$f(k, \hat{r}) = \sum_i f_i e^{ik\mathbf{r_i} \cdot \hat{\mathbf{r}}}. \tag{64}$$

The s-wave component of this scattering amplitude is

$$f_s(k) = \int \frac{d\Omega}{4\pi} f(k) = \sum_i f_i \frac{\sin kr_i}{kr_i}. \tag{65}$$

In particular, when $kr_i \ll 1$ then

$$f_s(k) = \sum_i f_i. \tag{66}$$

My goal is to calculate the phase shift δ given by

$$f_s = \frac{e^{i\delta} \sin \delta}{k}. \tag{67}$$

I now determine the f_i's via the restriction that at each impurity, the phase shift is δ_0. Once we know f_i we know f. Near the ith impurity, the spherically symmetric part of ψ is defined by

$$\psi_i^{(s)}(|\mathbf{r} - \mathbf{r_i}|) = \int \frac{d\Omega'}{4\pi} \psi(\mathbf{r} = \mathbf{r'} + \mathbf{r_i}), \tag{68}$$

where $d\Omega'$ is a solid angle with respect to the variable r', which is centered at the impurity. The integration is straight forward and one finds

$$\psi_i^{(s)}(r - r_i) = \left(e^{ikz_i} + \sum_{j, j \neq i} f_j \frac{e^{ik|r_i - r_j|}}{|r_i - r_j|} \right) \frac{\sin k|r - r_i|}{k|r - r_i|} + f_i \frac{e^{ik|r-r_i|}}{|r-r_i|}. \tag{69}$$

I will use the symbol A_i for the term in large parentheses. We know that this term must have the form

$$\psi_i^{(s)}(r - r_i) = \frac{\sin(k|r - r_i| + \delta_0)}{k|r - r_i|}. \tag{70}$$

Equating these two expressions, one arrives at

$$f_i = A_i \frac{e^{i\delta_0} \sin \delta_0}{k}. \tag{71}$$

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Using this expression in the definition of A_i one finds that A_i satisfies the following matrix equation,

$$\left(\delta_{ij} - e^{i\delta_0} \sin \delta_0 \frac{e^{ik|r_i - r_j|}}{k|r_i - r_j|} \right) A_j = e^{ikz_j}. \tag{72}$$

I denote the matrix on the left hand side of this equation by $1 - g$. Formally inverting this matrix gives

$$\begin{pmatrix} A_1 \\ \vdots \\ A_n \end{pmatrix} = \frac{1}{1 - g} \begin{pmatrix} e^{ikz_1} \\ \vdots \\ e^{ikz_n} \end{pmatrix}. \tag{73}$$

The total scattering amplitude f is then

$$f(k, \hat{k}, \hat{r}) = \frac{e^{i\delta_0} \sin \delta_0}{k} \begin{pmatrix} e^{-ik\hat{\mathbf{r}} \cdot \mathbf{r_1}} & \cdots & e^{-ik\hat{\mathbf{r}} \cdot \mathbf{r_n}} \end{pmatrix} \frac{1}{1 - g} \begin{pmatrix} e^{ik\hat{\mathbf{k}} \cdot \mathbf{r_1}} \\ \vdots \\ e^{ik\hat{\mathbf{k}} \cdot \mathbf{r_n}} \end{pmatrix} \tag{74}$$

$$= \frac{e^{i\delta_0} \sin \delta_0}{k} \sum_{ij} e^{ik(\hat{\mathbf{k}} \cdot \mathbf{r_i} - \hat{\mathbf{r}} \cdot \mathbf{r_j})} \left(\frac{1}{1 - g} \right)_{ij}. \tag{75}$$

Formally we are now done. If $kr_i \ll 1$ we neglect the e^{ikr_i}'s and get

$$e^{i\delta} \sin \delta = e^{i\delta_0} \sin \delta_0 \sum_{ij} \left(\frac{1}{1 - g} \right)_{ij}. \tag{76}$$

In this same approximation

$$g_{ij} = \begin{cases} \frac{e^{i\delta_0} \sin \delta_0}{k|r_i - r_j|} & i \neq j \\ 0 & i = j. \end{cases} \tag{77}$$

In the pseudo-potential approximation,

$$e^{i\delta_0} \sin \delta_0 = \frac{-a_s k}{1 + ia_s k}. \tag{78}$$

It is useful to study the structure of $(1 - g)^{-1}$. The matrix g has the property that g_{ij} is a function only of the distance $|r_i - r_j|$, and is essentially a scattering amplitude times a propegator. One graphically thinks of g_{ij} as a directed line connecting impurity i to impurity j. Then $((1 - g)^{-1})_{ij}$ is the sum over all paths connecting i to j.

7.2 T-matrix approach

With less work (but using more machinery) one can derive the results as the last Section by directly calculating the T-matrix, defined by

$$T = V + V \frac{1}{H_0 - E} T. \tag{79}$$

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In the present case, $V = \sum_i V_i$ is the sum of the potentials for each scatterer. If one defines T_i as the sum of scattering off an individual impurity,

$$T_i = V_i + V_i \frac{1}{H_0 - E} T_i, \tag{80}$$

then T is given by a sum over all paths between scatters of T_i's with propegators between them,

$$T = \sum_i T_i + \sum_{i \neq j} T_i \frac{1}{H_0 - E} T_j + \cdots, \tag{81}$$

$$= \sum_i T_i + \sum_{ij} T_i (1 - \delta_{ij}) \frac{1}{H_0 - E} T_j + \cdots. \tag{82}$$

I introduce a matrix G_{ij} by

$$G_{ij} = (1 - \delta_{ij}) \frac{1}{H_0 - E} T_j, \tag{83}$$

so that the T-matrix is formally

$$T = \sum_{ij} T_i \left(\frac{1}{1 - G} \right)_{ij}. \tag{84}$$

To go any farther one needs to choose a basis. The most convenient basis for the current problem is in momentum space. If we treat the T_i's within the pseudo-potential approximation, then

$$T_i(k, k', q) = \langle k' | T_i(E = q^2/2m) | k \rangle = e^{i(k-k')r_i} \left(\frac{-2\pi}{mq} e^{i\delta_0} \sin \delta_0 \right). \tag{85}$$

For notational simplicity, I use the symbol x for the parentheses. The operator $T_i(H_0 - E)^{-1} T_j$ is evaluated by inserting a resolution of the identity

$$\langle k' | T_i(H_0 - E)^{-1} T_j | k \rangle = \int \frac{d^3 \bar{k}}{(2\pi)^3} T(k, \bar{k}, q) \frac{2m}{\bar{k}^2 - q^2} T(\bar{k}, k', q) \tag{86}$$

$$= x^2 e^{i(kr_j - k'r_i)} \frac{m}{2\pi} \frac{e^{iq|r_i - r_j|}}{q|r_i - r_j|}. \tag{87}$$

In Eq. (81) all of the $e^{i\bar{k}r_i}$'s cancel, except for the one at the end and the one at the beginning. Thus T is given by

$$T(k, k', q) = x \sum_{ij} e^{i(kr_i - k'r_j)} M_{ij}(q), \tag{88}$$

where $M_{ij}(q)$ is the sum of all paths going from i to j, each segment of the path going from impurity μ to impurity ν contributing $x(m/2\pi)e^{iq|r_\mu - r_\nu|}/(q|r_\mu - r_\nu|)$, which is readily seen to be identical to (75).

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7.3 Two scatterers

Given the positions $\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_n}$ of the scatterers we can now calculate δ in terms of δ_0. The simplest example of this procedure uses two scatterers. The matrix g_{ij} is given by

$$g = \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix} \tag{89}$$

$$x = \frac{e^{ik|r_1 - r_2|}}{k|r_1 - r_2|} \sin \delta_0 e^{i\delta_0} \tag{90}$$

$$\approx \frac{-a_s(1 + ikr)/r}{1 + ika_s}, \tag{91}$$

where $r \equiv |r_1 - r_2|$ and a_s is the scattering length for scattering off a single impurity. Since g is proportional to a Pauli matrix, $g^2 = x^2$ is proportional to the identity. Thus $(1 - g)^{-1}$ is $(1 - x^2)^{-1}(1 + g)$. The scattering amplitude is then

$$f = \frac{e^{i\delta_0} \sin \delta_0}{k} \sum_{ij} \left(\frac{1}{1 - g} \right)_{ij} \tag{92}$$

$$= \frac{e^{i\delta_0} \sin \delta_0}{k} \frac{1}{1 - x^2} (2 + 2x) \tag{93}$$

$$= \frac{-\left(\frac{2a_s}{1 + a_s/r} \right)}{1 + i \left(\frac{2a_s}{1 + a_s/r} \right) k}. \tag{94}$$

The last line follows from some simple algebraic rearrangements. The end result is that the scattering from two impurities looks like scattering from a single one with an effective scattering length

$$a_2 = \frac{2a_s}{1 + a_s/r}. \tag{95}$$

For $a_s \ll r$ the scattering is just additive. For $a_s \gg r$ the effective scattering length is cut off by the distance between the two impurities, and $a_2 \to 2r$.

It should be clear from this result that when particles are packed closer than their scattering lengths one cannot consider the scattering from each particle independently.

7.4 Low density limit

In the low density limit, $na_s^3 \ll 1$, the matrix elements g_{ij} are small, and the single scattering dominates. The phase shift for scattering off the collection of impurities is then additive, $\delta = N\delta_0$.

8 Scattering in the many body problem

For information on the many-body problem please refer to my thesis.

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