Advanced quantum mechanics

Chapter 4 – Describing interactions: quantum scattering

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Outline

1. Quantum scattering
   - The two-body problem
   - The Lippmann–Schwinger equation
   - Born approximation and perturbative expansion
   - Partial wave decomposition
   - Scattering between identical particles
   - Examples
   - Scattering resonances
   - The Fermi–Huang pseudopotential

Chapter 4 – Describing interactions

A many-body Hamiltonian contains single-particle terms (kinetic energy, external potential) and binary interactions between pairs of particles.

- Interactions are characterized by the two-body scattering problem.
- Scattering is also the main experimental probe of matter: from Rutherford's discovery of the nucleus to particle colliders, and neutron, electron or X-ray scattering in condensed matter.
- At low energy, the details of the potential become irrelevant: a single parameter, the scattering length a, suffices.
- This leads to the zero-range pseudopotential, used throughout the rest of the course (Bogoliubov and BCS theories).

Genuine three-body interactions, relevant in more exotic systems, are not considered.

Center-of-mass and relative motions

Two particles of masses m_1, m_2:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V(\hat{\mathbf{r}}_2 - \hat{\mathbf{r}}_1), \qquad V(\mathbf{r}) \xrightarrow[r\to\infty]{} 0.$$

Translation invariance separates the motions. With

$$\hat{\mathbf{R}} = \frac{m_1\hat{\mathbf{r}}_1 + m_2\hat{\mathbf{r}}_2}{M}, \quad \hat{\mathbf{P}} = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2, \qquad \hat{\mathbf{r}} = \hat{\mathbf{r}}_2 - \hat{\mathbf{r}}_1, \quad \hat{\mathbf{p}} = \mu\left(\frac{\hat{\mathbf{p}}_2}{m_2} - \frac{\hat{\mathbf{p}}_1}{m_1}\right),$$

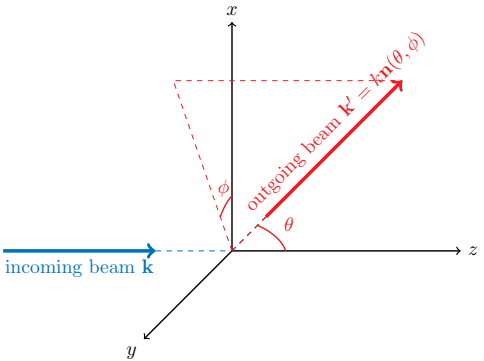
where $M = m_1 + m_2$ and $\mu = m_1 m_2/M$ is the reduced mass,

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2\mu} + V(\hat{\mathbf{r}}), \qquad |\Psi\rangle = |\mathbf{P}\rangle \otimes |\psi\rangle.$$

A fictitious particle of mass μ in the potential $V(\mathbf{r})$, with

- discrete bound states of energy $E < 0$,
- a continuum of scattering states of energy $E > 0$ — the subtle case.

Scattering cross-section



A beam of incoming flux j along $\mathbf{e}_z$ hits a target. We consider elastic scattering: same internal state, same kinetic energy.

Total cross-section: rate of scattered particles

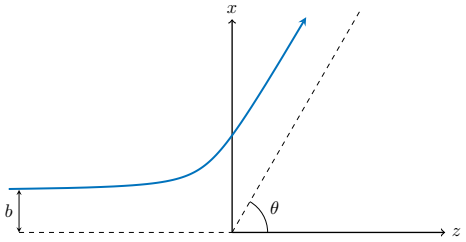
$$\dot{N} = j\,\sigma.$$

Differential cross-section: rate towards the direction $\mathbf{n} = (\theta, \phi)$, within the solid angle $\mathrm{d}^2\Omega$,

$$\mathrm{d}\dot{N} = j \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \right) \mathrm{d}^2\Omega.$$

The polar angle θ is measured from the incident beam axis.

Reminder: classical scattering



For an isotropic potential, a trajectory of impact parameter b exits at the angle $\theta(b)$ [1]:

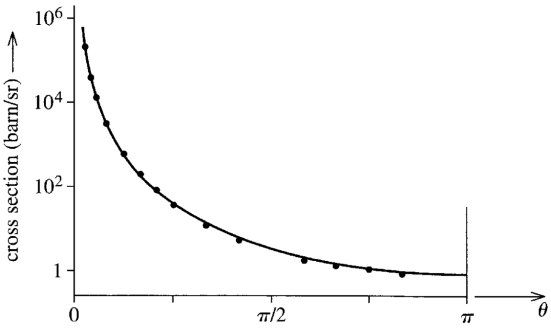
$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \left|\frac{\mathrm{d}(\pi b^2)}{\mathrm{d}[2\pi(1-\cos\theta)]}\right| = \frac{1}{4}\left|\frac{\mathrm{d}b^2}{\mathrm{d}\sin^2(\theta/2)}\right|.$$

Hard sphere of radius R: isotropic,

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \frac{R^2}{4}, \qquad \sigma = \pi R^2,$$

the geometric cross-section.

Reminder: Rutherford scattering



Alpha particles on gold nuclei, Coulomb potential $V(r) = qQ/(4\pi\varepsilon_0 r)$:

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \left(\frac{qQ}{16\pi\varepsilon_0 E \sin^2(\theta/2)}\right)^2 .$$

Tested with great accuracy by Geiger and Marsden: strong support for Rutherford's planetary model of the atom.

We will recover this formula from quantum mechanics, within the Born approximation.

Quantum scattering states

Stationary state of energy $E = \hbar^2 k^2/(2\mu) > 0$,

$$E\psi_{\mathbf{k}}(\mathbf{r}) = \left[-\frac{\hbar^2}{2\mu}\Delta + V(\mathbf{r})\right]\psi_{\mathbf{k}}(\mathbf{r}), \qquad \psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + \psi_{\mathrm{sc}}(\mathbf{r}), \quad \mathbf{k} = k\,\mathbf{e}_z.$$

In the far field ($r \gg b$, the potential range), the scattered wave is an outgoing spherical wave

$$\psi_{\mathrm{sc}}(\mathbf{r}) \simeq f(\mathbf{k},\mathbf{k}')\,\frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \qquad \mathbf{k}' = k\,\mathbf{n}: \text{ the scattering amplitude.}$$

Probability current $\mathbf{j} = \frac{\hbar}{2\mu\mathrm{i}}(\psi^*\nabla\psi - \psi\nabla\psi^*)$:

- incoming flux $\mathbf{j}_{\mathrm{in}} = \hbar\mathbf{k}/\mu$;
- scattered flux $\mathbf{j}_{\mathrm{sc}} = \frac{\hbar k}{\mu}\frac{|f|^2}{r^2}\,\mathbf{n}$;
- cross terms oscillate as $\mathrm{e}^{\pm\mathrm{i}kr(1-\cos\theta)}$ and average out, except in the forward direction.

$$\mathbf{j}_{\mathrm{sc}}\cdot\mathbf{n}\; r^2\mathrm{d}^2\Omega = j_{\mathrm{in}}|f|^2\mathrm{d}^2\Omega \quad\Longrightarrow\quad \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = |f(\mathbf{k},\mathbf{k}')|^2$$

The Lippmann–Schwinger equation

Treat the potential as a source term:

$$\frac{\hbar^2}{2\mu}(\Delta + k^2)\psi_{\mathbf{k}}(\mathbf{r}) = V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}).$$

Green function $\frac{\hbar^2}{2\mu}(\Delta + k^2)\mathcal{G}_0(\mathbf{r}) = \delta(\mathbf{r})$: incoming or outgoing spherical waves,

$$\mathcal{G}_0^{(\pm)}(\mathbf{r}) = -\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\pm \mathrm{i}kr}}{r}.$$

Keeping only the outgoing wave [2]:

Lippmann–Schwinger equation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + \int \mathcal{G}_0^{(+)}(\mathbf{r} - \mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}^3r'$$

Not an explicit solution: $\psi_{\mathbf{k}}$ appears under the integral. But a natural starting point for approximations.

Scattering amplitude and transition matrix

Far field: $|\mathbf{r}-\mathbf{r}'| \simeq r - \mathbf{n}\cdot\mathbf{r}'$, hence

$$\psi_{\mathbf{k}}(\mathbf{r}) \simeq \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} - \frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\int \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{r}'} V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,\mathrm{d}^3r'.$$

Conventions (as in the rest of the course): plane waves in a box of volume L^3, $\langle\mathbf{r}|\mathbf{k}\rangle = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}/L^{3/2}$, $\sum_{\mathbf{k}} \to L^3\int \frac{\mathrm{d}^3k}{(2\pi)^3}$; $|\psi_{\mathbf{k}}\rangle$ normalized like $|\mathbf{k}\rangle$.

Transition operator: $\hat{T}|\mathbf{k}\rangle = \hat{V}|\psi_{\mathbf{k}}\rangle$. Matrix elements scale as $1/L^3$: we use the box-independent

$$\tilde{V}(\mathbf{k}'-\mathbf{k}) \equiv L^3\langle\mathbf{k}'|\hat{V}|\mathbf{k}\rangle = \int \mathrm{e}^{-\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} V(\mathbf{r})\,\mathrm{d}^3r, \qquad \mathcal{T}(\mathbf{k}',\mathbf{k}) \equiv L^3\langle\mathbf{k}'|\hat{T}|\mathbf{k}\rangle,$$

$$f(\mathbf{k},\mathbf{k}') = -\frac{\mu}{2\pi\hbar^2}\,\mathcal{T}(\mathbf{k}',\mathbf{k}).$$

From now on, L no longer appears: the formulas are those obtained with plane waves $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$.

The Born approximation

Lowest order in V: replace $\psi_{\mathbf{k}}$ by the incoming plane wave in the Lippmann–Schwinger equation,

Born approximation

$$f(\mathbf{k}, \mathbf{k}') = -\frac{\mu}{2\pi\hbar^2}\,\tilde{V}(\mathbf{q}), \qquad \mathbf{q} = \mathbf{k}' - \mathbf{k} \text{ (momentum transfer)}.$$

The scattering amplitude is the Fourier transform of the potential. Equivalently: Fermi's golden rule between $|\mathbf{k}\rangle$ and the continuum $|\mathbf{k}'\rangle$.

Validity. For a potential of magnitude $|V_0|$ and range b:

$$|V_0| \ll \frac{\hbar^2}{\mu b^2} \;\; \text{(low energy, } kb \lesssim 1), \qquad |V_0|\, b \ll \hbar v = \frac{\hbar^2 k}{\mu} \;\; \text{(high energy, } kb \gg 1).$$

- The first condition: the potential is too weak to bind a particle.
- The second: the Born approximation always becomes valid at high enough energy.

Example: Yukawa and Coulomb potentials

Yukawa potential — nuclear forces (pion exchange), screened Coulomb interaction in solids:

$$V(r) = \alpha \frac{\mathrm{e}^{-r/R}}{r} \quad \Longrightarrow \quad \tilde{V}(\mathbf{q}) = \frac{4\pi\alpha R^2}{1+q^2R^2}, \qquad q = 2k\sin(\theta/2).$$

Hence

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \left(\frac{2\alpha\mu}{\hbar^2}\,\frac{R^2}{1+4k^2R^2\sin^2(\theta/2)}\right)^2.$$

Coulomb limit $R \to \infty$, $\alpha = qQ/(4\pi\varepsilon_0)$:

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \left(\frac{\alpha\mu}{2\hbar^2k^2\sin^2(\theta/2)}\right)^2 = \left(\frac{qQ}{16\pi\varepsilon_0 E\sin^2(\theta/2)}\right)^2.$$

The Rutherford formula is recovered — remarkably, $\hbar$ drops out.

Example: Bragg scattering

A periodic potential has a discrete Fourier spectrum, on the reciprocal lattice

$$\mathbf{g} = n_1\mathbf{g}_1 + n_2\mathbf{g}_2 + n_3\mathbf{g}_3, \qquad n_i \in \mathbb{Z}.$$

Scattering only occurs towards $\mathbf{k}' = \mathbf{k} + \mathbf{g}$, with the elastic condition $|\mathbf{k}'| = k$:

$$2\mathbf{k}\cdot\mathbf{g} + g^2 = 0 \qquad \text{(Laue condition } \Leftrightarrow \text{ Bragg's law)}.$$

Generically violated: diffraction peaks require specific crystal orientations, a polychromatic beam, or a powder.

Quasicrystals. Bragg diffraction only requires a discrete Fourier spectrum,

$$\mathbf{g} = \sum_{i=1}^{p} n_i\mathbf{g}_i,$$

with p incommensurate vectors, p larger than the dimension. Sharp diffraction peaks without periodicity: quasi-crystalline order [3].

Operator form: the resolvent

With $\hat{H}_0 = \hat{p}^2/(2\mu)$: $(E - \hat{H}_0)|\psi_{\mathbf{k}}\rangle = \hat{V}|\psi_{\mathbf{k}}\rangle$. Not invertible for $E > 0$: regularize with $\mathrm{i}\eta$, $\eta \to 0^+$,

$$|\psi_{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \hat{G}_0^{(+)}\hat{V}|\psi_{\mathbf{k}}\rangle, \qquad \hat{G}_0^{(+)} = \frac{1}{E - \hat{H}_0 + \mathrm{i}\eta} \quad \text{(resolvent, Chapter 1)}.$$

In position space, $\langle \mathbf{r}'|\hat{G}_0^{(+)}|\mathbf{r}\rangle$ solves the Green equation with $k \to k + \mathrm{i}\eta'$:

$$\mathcal{G}_0(r) = A_- \frac{\mathrm{e}^{-\mathrm{i}(k+\mathrm{i}\eta')r}}{r} + A_+ \frac{\mathrm{e}^{\mathrm{i}(k+\mathrm{i}\eta')r}}{r}.$$

The incoming wave diverges as $\mathrm{e}^{\eta' r}$, hence $A_- = 0$.

The sign of $\mathrm{i}\eta$ selects the outgoing spherical wave: $\langle \mathbf{r}'|\hat{G}_0^{(+)}|\mathbf{r}\rangle = \mathcal{G}_0^{(+)}(|\mathbf{r} - \mathbf{r}'|)$.

The Born series

Iterating,

$$|\psi_{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \hat{G}_0^{(+)}\hat{V}|\mathbf{k}\rangle + (\hat{G}_0^{(+)}\hat{V})^2|\mathbf{k}\rangle + \ldots = |\mathbf{k}\rangle + \hat{G}_0^{(+)}\hat{T}|\mathbf{k}\rangle,$$

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0^{(+)}\hat{V} + \hat{V}(\hat{G}_0^{(+)}\hat{V})^2 + \ldots$$

A sum over sequences of elementary scattering events. At second order, via intermediate momenta $\mathbf{k}''$:

$$\mathcal{T}(\mathbf{k}', \mathbf{k}) = \tilde{V}(\mathbf{k}' - \mathbf{k}) + \int \frac{\tilde{V}(\mathbf{k}' - \mathbf{k}'')\tilde{V}(\mathbf{k}'' - \mathbf{k})}{E - \hbar^2 k''^2/(2\mu) + \mathrm{i}\eta} \frac{\mathrm{d}^3 k''}{(2\pi)^3} + \ldots$$

Convergence [4]:

- converges above some energy E_*, for a potential decaying fast enough;
- converges at all energies if $-|V|$ has no bound state;
- diverges at low energy if V has a bound state: no finite order reproduces the pole of f.

Example: van der Waals interaction between cold atoms, with dozens of bound states.

Partial waves

For a spherically symmetric $V(r)$, decompose on angular momentum. Plane wave along $\mathbf{e}_z$:

$$e^{ikz} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr) P_\ell(\cos\theta) \underset{kr\gg 1}{\simeq} \frac{1}{2ikr} \sum_{\ell=0}^{\infty} (2\ell+1) \left[(-1)^{\ell+1} e^{-ikr} + e^{ikr}\right] P_\ell(\cos\theta),$$

with $P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell 0}(\theta)$: only $m = 0$ appears.

Rotational symmetry: an incoming wave ℓ is scattered into an outgoing wave of the *same* ℓ,

$$\psi_{\mathbf{k}}(\mathbf{r}) \simeq \frac{1}{2ikr} \sum_{\ell=0}^{\infty} (2\ell+1) \left[(-1)^{\ell+1} e^{-ikr} + S_\ell\, e^{ikr}\right] P_\ell(\cos\theta).$$

Flux conservation (elastic scattering): $|S_\ell| = 1$,

$$S_\ell = e^{2i\delta_\ell} : \text{ scattering phase shifts.}$$

Channels $\ell = 0, 1, 2, \ldots$ are called $s, p, d, \ldots$ waves.

Cross-section and unitary limit

Scattering amplitude, independent of ϕ:

$$f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\delta_\ell} - 1) P_\ell(\cos\theta).$$

Orthogonality of the Legendre polynomials separates the partial waves:

$$\sigma = \sum_\ell \sigma_\ell, \qquad \sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell \;\leq\; \sigma_\ell^{\max} = \frac{4\pi}{k^2}(2\ell+1),$$

the unitary limit, reached for $\delta_\ell = \pi/2 \pmod{\pi}$.

Optical theorem

Using $P_\ell(1) = 1$:

$$\operatorname{Im} f(\theta = 0) = \frac{k}{4\pi}\,\sigma.$$

Conservation of probability: the interference between the incoming and scattered waves in the forward direction removes exactly the flux scattered in all other directions.

Radial equation and bound states

Writing $\psi = Y_\ell^m(\theta,\phi)\, u_\ell(r)/r$:

$$u_\ell''(r) + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu V(r)}{\hbar^2}\right] u_\ell(r) = 0, \qquad u_\ell(0) = 0,$$

whose large-r behaviour gives the phase shift:

$$u_\ell(r) \propto (-1)^{\ell+1} \mathrm{e}^{-\mathrm{i}kr} + \mathrm{e}^{2\mathrm{i}\delta_\ell} \mathrm{e}^{\mathrm{i}kr} \propto \sin(kr - \ell\pi/2 + \delta_\ell).$$

Bound states. A bound state of energy $E = -\hbar^2 q^2/(2\mu)$ decays as e^{-qr}/r:

- an outgoing wave $\mathrm{e}^{\mathrm{i}kr}/r$ with an imaginary wave-vector $k = \mathrm{i}q$;
- with no incoming wave, i.e. an infinite scattering amplitude.

bound states $\Leftrightarrow$ poles of f (or S_ℓ) on the positive imaginary axis $k \in \mathrm{i}\mathbb{R}_+$

Low energy: the centrifugal barrier

For $\ell \geq 1$, the centrifugal barrier suppresses the wave-function for

$$r < r_E = \sqrt{\frac{\hbar^2 \ell(\ell+1)}{2\mu E}}.$$

When r_E exceeds the range b, the potential is not felt: $\delta_\ell \to 0$.

More precisely, for $r > b$, $u_\ell = A\sqrt{kr}J_{\ell+1/2}(kr) + B\sqrt{kr}Y_{\ell+1/2}(kr)$:

- $r \gg 1/k$: $u_\ell \simeq \sqrt{2/\pi}\,[A\sin(kr - \ell\pi/2) - B\cos(kr - \ell\pi/2)]$, so $B/A = -\tan\delta_\ell$;
- $b \ll r \ll 1/k$: $u_\ell \propto c_1 A\, r^{\ell+1} + c_2 \dfrac{B}{k^{2\ell+1}}\, r^{-\ell}$, fixed by the zero-energy solution, *independent of* k.

$$\tan\delta_\ell(k) \propto k^{2\ell+1} \qquad (k \to 0)$$

At low energy, only a few partial waves contribute: this is the interest of the decomposition.
Valid for potentials decaying faster than $1/r^{2\ell+3}$. For van der Waals ($1/r^6$), $\tan\delta_\ell \propto k^4$ for all $\ell \geq 2$.

The scattering length

Cold collision regime: only the s wave contributes, and scattering is isotropic. It is characterized by the scattering length

$$a = -\lim_{k\to 0} \frac{\tan\delta_0(k)}{k} \qquad \Longrightarrow \qquad f = \frac{e^{2i\delta_0}-1}{2ik} \simeq -\frac{a}{1+ika}, \qquad \sigma = \frac{4\pi a^2}{1+k^2a^2}.$$

At zero energy, $u_0(r) \propto r - a$ outside the potential. a can be positive, negative, or infinite ($\delta_0 \to \pi/2$).

Weakly bound state. Pole at $k = i/a$, on $i\mathbb{R}_+$ for $a > 0$:

$$E = -\frac{\hbar^2}{2\mu a^2}, \qquad \psi \propto \frac{e^{-r/a}}{r}.$$

- Meaningful only if $a \gg b$. Counter-example: the hard sphere has $a = R > 0$ but no bound state.
- Deeper bound states may exist outside the low-energy regime.
- Each new bound state appears at threshold, where a diverges. Levinson's theorem: $\delta_0(0) - \delta_0(\infty) = N_b\pi$.

When is the cold collision regime reached?

Neutrons. Nuclear interaction of range $b \simeq 2\,\mathrm{fm}$:

$$E \ll E_\star = \frac{\hbar^2}{2\mu b^2} = \frac{\hbar^2}{m_n b^2} \simeq 10\,\mathrm{MeV}.$$

Fulfilled by slow neutron beams and in neutron stars. With no free neutron target, a_{nn} is measured from reactions with two neutrons in the final state, e.g. $\pi^- + d \to n + n + \gamma$ [5]:

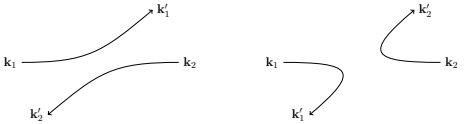
$$a_{nn} \simeq -18.6\,\mathrm{fm}.$$

Neutral atoms. Van der Waals tail $V(r) = -C_6/r^6$. Dimensional analysis:

$$R_{\mathrm{vdW}} = \left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}, \qquad E_\star = \frac{\hbar^2}{2\mu R_{\mathrm{vdW}}^2} \sim k_B \times 100\,\mu\mathrm{K} \quad \text{(alkali atoms)}.$$

Ultracold gases ($T \lesssim 1\,\mu\mathrm{K}$) are deep in the cold collision regime: their interactions are fully characterized by a.

Identical particles



Same internal state. The center-of-mass motion is symmetric, so the relative wave-function carries the exchange symmetry ($\mathbf{r} \to -\mathbf{r}$):

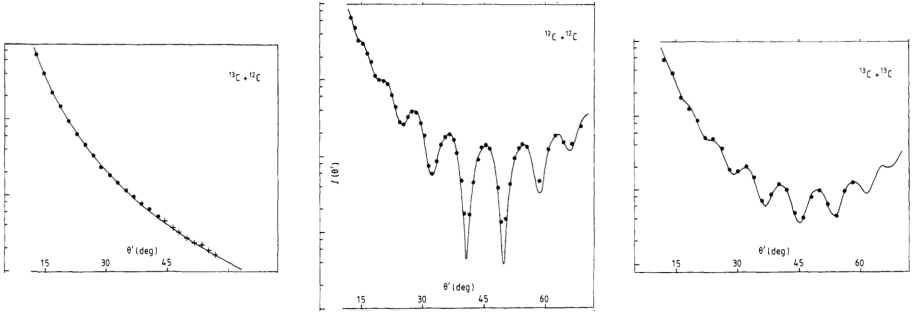
$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{2}}\left(e^{i\mathbf{k}\cdot\mathbf{r}} + \varepsilon\, e^{-i\mathbf{k}\cdot\mathbf{r}} + [f(\mathbf{k},\mathbf{k}') + \varepsilon f(\mathbf{k},-\mathbf{k}')]\frac{e^{ikr}}{r}\right),$$

$\varepsilon = +1$ (bosons), -1 (fermions). Two indistinguishable processes interfere:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}|f(\mathbf{k},\mathbf{k}') + \varepsilon\, f(\mathbf{k},-\mathbf{k}')|^2.$$

- At 90°, $f(\mathbf{k},\mathbf{k}') = f(\mathbf{k},-\mathbf{k}')$: constructive for bosons, destructive for fermions.
- Compare with the incoherent sum $\frac{1}{2}\left(|f(\mathbf{k},\mathbf{k}')|^2 + |f(\mathbf{k},-\mathbf{k}')|^2\right)$.

Collisions between carbon isotopes



^{12}C (boson) and ^{13}C (spin-1/2 fermion) beams on targets at rest [6]. Different isotopes: Rutherford. Identical isotopes: interferences.

- 90° in the center-of-mass frame $= 45^\circ$ in the laboratory frame (equal masses).
- Unpolarized ^{13}C: singlet (1/4, symmetric orbital) and triplet (3/4, antisymmetric orbital),

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{2}\left(|f(\mathbf{k},\mathbf{k}')|^2 + |f(\mathbf{k},-\mathbf{k}')|^2 - \mathrm{Re}[f(\mathbf{k},\mathbf{k}')f^*(\mathbf{k},-\mathbf{k}')]\right) :$$

destructive interference with half the contrast.

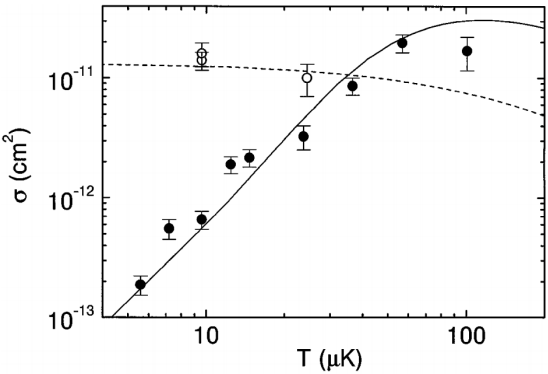
Statistics and partial waves

A partial wave ℓ has parity $(-1)^\ell$:

- identical bosons: even ℓ only;
- identical fermions: odd ℓ only.

In the cold collision regime, spin-polarized fermions do not interact: the lowest allowed channel is *p*-wave, suppressed by the centrifugal barrier.

Observed with ^{40}K: the collision rate of a spin-polarized gas vanishes at low temperature, unlike that of a spin mixture [7].



Hard-sphere potential

$V = +\infty$ for $r < R$, 0 otherwise: boundary condition $u_\ell(R) = 0$. For $r > R$,

$$u_\ell(r) = A_\ell \left[\cos\delta_\ell \sqrt{kr} J_{\ell+1/2}(kr) - \sin\delta_\ell \sqrt{kr} Y_{\ell+1/2}(kr) \right] \underset{kr \gg 1}{\propto} \sin(kr - \ell\pi/2 + \delta_\ell),$$

hence

$$\tan\delta_\ell = \frac{J_{\ell+1/2}(kR)}{Y_{\ell+1/2}(kR)}.$$

s **wave:** $u_0 \propto \sin[k(r-R)]$, so $\delta_0 = -kR$ exactly, and

$$a = R, \qquad \sigma = 4\pi R^2 \quad (k \to 0).$$

Four times the classical geometric cross-section πR^2: a wave (diffraction) effect.

More generally, a potential everywhere positive gives a positive scattering length.

Square-well potential

$V = -U$ for $r < R$, 0 otherwise, with $U = \hbar^2 k_0^2/(2\mu)$. Zero-energy s-wave state:

$$u_0(r) = A\sin(k_0 r) \quad (r < R), \qquad u_0(r) \propto r - a \quad (r > R).$$

Continuity of u_0 and u_0' at $r = R$:

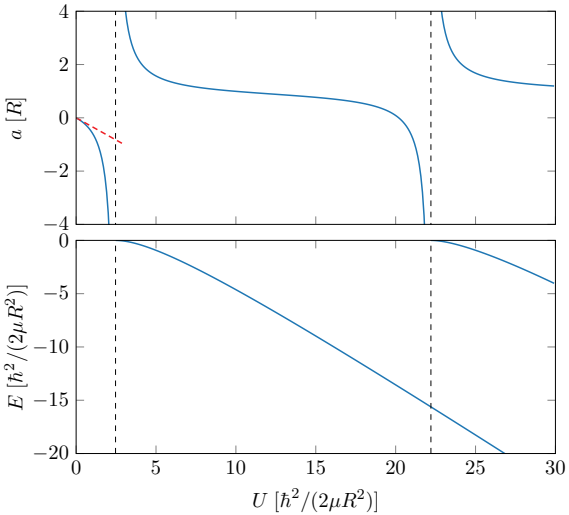
$$a = R - \frac{\tan(k_0 R)}{k_0}$$

- **Shallow well** $U \ll \hbar^2/(2\mu R^2)$: $a \simeq -k_0^2 R^3/3$, which coincides with the Born approximation

$$a = -f(0) = \frac{\mu}{2\pi\hbar^2}\int V(r)\,\mathrm{d}^3 r = -\frac{k_0^2 R^3}{3}.$$

- **Deeper wells**: a takes any value, positive or negative.
- **Resonances** at $k_0 R = (n + \frac{1}{2})\pi$: $a \to \pm\infty$, unitary limit $\sigma_0 = 4\pi/k^2$.

Square well: scattering length and bound states



Top: scattering length (blue), Born approximation (red dashed).

Bottom: bound state energies.

Each divergence of a coincides with the appearance of a new bound state at threshold, at $U = (n + \frac{1}{2})^2 \pi^2 \hbar^2/(2\mu R^2)$.

Just past a resonance (U slightly larger, $a \gg R$), the new bound state has the universal energy $-\hbar^2/(2\mu a^2)$.

The Born approximation fails as soon as the well can bind.

Bound states and virtual states

Resonances: strong enhancement of scattering due to a (quasi-)bound state close to the collision energy. Unified view: poles of $S_\ell(k)$ in the complex k plane.

Low-energy s wave:

$$S_0(k) = 1 + 2\mathrm{i}kf = \frac{1 - \mathrm{i}ka}{1 + \mathrm{i}ka}, \qquad \text{pole at } k = \mathrm{i}/a.$$

- $a > 0$: pole on $\mathrm{i}\mathbb{R}_+ \to$ bound state, $E = -\hbar^2/(2\mu a^2)$.
- $a < 0$: pole on $-\mathrm{i}\mathbb{R}_+ \to$ virtual state. The wave-function $\mathrm{e}^{r/|a|}/r$ diverges: not a state of the spectrum. Yet, if $|a| \gg b$, it strongly enhances low-energy scattering, $\sigma_0 = 4\pi a^2/(1 + k^2 a^2) \gg b^2$.

Example: two neutrons. $a_{nn} \simeq -18.6\,\mathrm{fm}$: no dineutron, but a virtual state at only

$$\frac{\hbar^2}{m_n a_{nn}^2} \simeq 0.1\,\mathrm{MeV} \ll E_\star \simeq 10\,\mathrm{MeV}.$$

Quasi-bound states: the Breit–Wigner formula

Pole close to the real axis, $k = k_r - \mathrm{i}\gamma$ $(0 < \gamma \ll k_r)$:

$$E \simeq E_r - \frac{\mathrm{i}\hbar\Gamma}{2}, \qquad E_r = \frac{\hbar^2 k_r^2}{2\mu}, \quad \Gamma = \frac{2\hbar k_r \gamma}{\mu} :$$

a quasi-bound state, trapped in the potential region for a lifetime $1/\Gamma$. Near E_r:

$$S_\ell(E) \simeq \mathrm{e}^{2\mathrm{i}\delta_{\mathrm{bg}}} \frac{E - E_r - \mathrm{i}\hbar\Gamma/2}{E - E_r + \mathrm{i}\hbar\Gamma/2}, \qquad \tan\delta_{\mathrm{res}} = \frac{\hbar\Gamma/2}{E_r - E}.$$

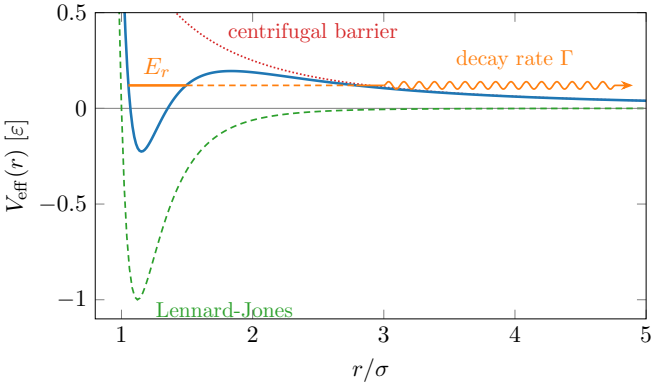
The phase shift increases by π across the resonance. For $\delta_{\mathrm{bg}} = 0$:

Breit–Wigner formula

$$\sigma_\ell(E) = \frac{4\pi}{k^2}(2\ell+1)\,\frac{(\hbar\Gamma/2)^2}{(E - E_r)^2 + (\hbar\Gamma/2)^2}$$

The same Lorentzian as for a discrete state decaying into a continuum (Wigner–Weisskopf, Chapter 1).

Shape resonances



For $\ell \geq 1$, the effective potential

$$V(r) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}$$

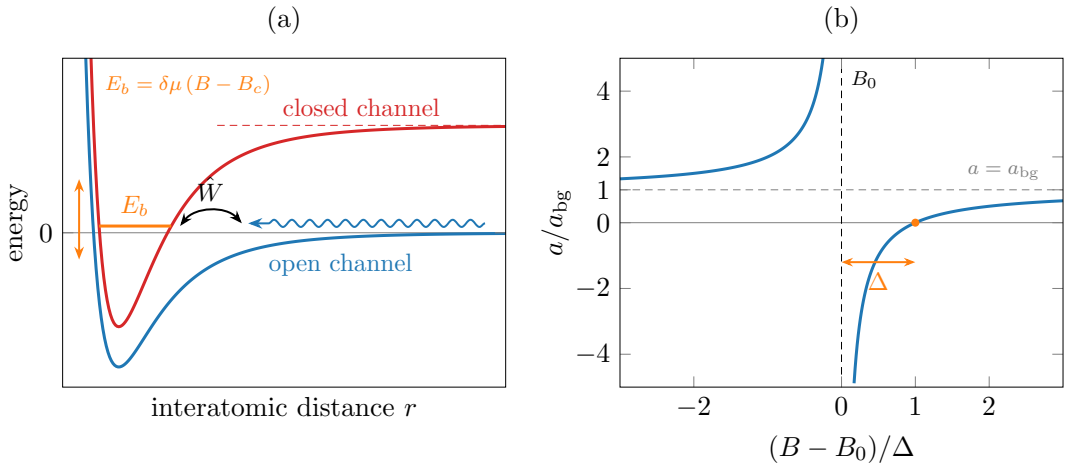
combines a short-range well and the centrifugal barrier.

A state of positive energy E_r can be trapped behind the barrier: a quasi-bound state, decaying by tunneling at the rate Γ.

Narrower at low energy, $\Gamma \propto k_r^{2\ell+1}$.

Here: Lennard-Jones potential, with $\hbar^2 \ell(\ell+1)/(2\mu\sigma^2) = \varepsilon$.

Feshbach resonances: the two-channel picture



(a) Atoms colliding in the open channel are coupled by $\hat{W}$ to a molecular state $|b\rangle$ of the closed channel, whose energy E_b is tuned by the magnetic field. (b) Resulting scattering length: divergence at B_0, zero crossing at $B_0 + \Delta$.

Feshbach resonances: mechanism

Coupling between internal states of the colliding atoms:

- open channel: incoming atoms, threshold $E = 0$;
- closed channel: higher threshold, but hosts a molecular state $|b\rangle$ of energy E_b close to 0.

Different magnetic moments: tunable with a magnetic field,

$$E_b(B) \simeq \delta\mu\,(B - B_c).$$

Eliminating the closed channel (effective Hamiltonian, Chapter 1):

$$\hat{V}_{\text{eff}}(E) = \hat{V}_{\text{bg}} + \frac{\hat{W}|b\rangle\langle b|\hat{W}}{E - E_b}.$$

Born approximation on the resonant term, at $E = 0$:

$$a - a_{\text{bg}} \simeq \frac{\mu}{2\pi\hbar^2}\frac{|W_0|^2}{-E_b}, \qquad W_0 = L^{3/2}\langle b|\hat{W}|\mathbf{k} = \mathbf{0}\rangle :$$

negative for $E_b > 0$, positive for $E_b < 0$, divergent when the molecular state crosses threshold.

Feshbach resonances: tuning the interactions

Generic form, confirmed by a full treatment [8]:

$$a(B) = a_{\mathrm{bg}}\left(1 - \frac{\Delta}{B - B_0}\right),$$

Δ: width; B_0: resonance position, shifted from B_c by the coupling.

- On the side $a \gg b$, the closed-channel state is dressed into a weakly bound Feshbach molecule, of universal energy $-\hbar^2/(2\mu a^2)$, mostly in the open channel.
- First observed in a sodium Bose–Einstein condensate [9].
- Now the main tool to tune interactions in ultracold gases, from strongly repulsive to strongly attractive.
- Broad resonance of ^{6}Li at $B_0 \simeq 832\,\mathrm{G}$: the workhorse of the BEC–BCS crossover (Chapter 7).

A zero-range model

In the cold collision regime, scattering depends on a only. Many potentials give the same a (e.g. the square well, for many (R, U)). We want a model with

- a single parameter,
- zero range: the low-energy form is *exact* for $r > 0$,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} - \frac{a}{1 + \mathrm{i}ka} \frac{\mathrm{e}^{\mathrm{i}kr}}{r}.$$

Reverse engineering. Free equation for $r > 0$, but $(\Delta + k^2)\mathrm{e}^{\mathrm{i}kr}/r = -4\pi\delta(\mathbf{r})$:

$$\left(-\frac{\hbar^2}{2\mu}\Delta - E\right)\psi_{\mathbf{k}} = -\frac{g}{1 + \mathrm{i}ka}\,\delta(\mathbf{r}), \qquad g = \frac{2\pi\hbar^2 a}{\mu}.$$

V must compensate this term: $V[\psi] = g\,\delta(\mathbf{r})\,L[\psi]$ with $L[\psi_{\mathbf{k}}] = \frac{1}{1+\mathrm{i}ka}$ for all k.

Wrong candidate: $g\,\delta(\mathbf{r})$, i.e. $L[\psi] = \psi(\mathbf{0})$: infinite, and no k-dependence.

The Fermi–Huang pseudopotential

Short-distance expansion of the scattering state:

$$\psi_{\mathbf{k}} = \frac{c}{r} + B + O(r), \qquad c = -\frac{a}{1+\mathrm{i}ka}, \qquad B = \frac{1}{1+\mathrm{i}ka} : \text{ the required weight!}$$

Fermi–Huang pseudopotential [10]

$$V_{\mathrm{pp}}[\psi(\mathbf{r})] = g\,\delta(\mathbf{r})\frac{\partial(r\psi(\mathbf{r}))}{\partial r} \qquad \text{i.e.} \qquad \psi = \frac{c}{r} + \psi_{\mathrm{reg}} \;\Rightarrow\; V_{\mathrm{pp}}[\psi] = g\,\psi_{\mathrm{reg}}(\mathbf{0})\,\delta(\mathbf{r}),$$

$$g = \frac{2\pi\hbar^2 a}{\mu} \quad (= 4\pi\hbar^2 a/m \text{ for identical particles}).$$

- Acts as a delta potential on regular functions ($c = 0$).
- Bethe–Peierls boundary condition $c = -aB$: $\psi \propto 1 - a/r$, i.e. $u(r) \propto r - a$ at short distance. Unique once restricted to this domain [11].
- **Bound state**: $\mathrm{e}^{-qr}/r = 1/r - q + \ldots$ satisfies it for $q = 1/a$. A single bound state for $a > 0$, $E = -\hbar^2/(2\mu a^2)$; none for $a < 0$.

The pseudopotential in momentum space

Not a multiplicative potential: a separable operator $V_{\text{pp}}[\psi] = g\,\delta(\mathbf{r})\,L[\psi]$, with $L[\psi] = \psi_{\text{reg}}(\mathbf{0})$. In Fourier space:

$$L[\psi] = \int \Lambda(k)\,\tilde{\psi}(\mathbf{k})\,\frac{\mathrm{d}^3k}{(2\pi)^3}.$$

- Regular ψ: $L[\psi] = \psi(\mathbf{0}) = \int \tilde{\psi} \Rightarrow \Lambda(k) = 1$ at finite k (as for $g\,\delta(\mathbf{r})$).
- $L[1/r] = 0$, with $\widetilde{1/r} = 4\pi/k^2 \Rightarrow \int_0^\infty \Lambda(k)\,\mathrm{d}k = 0$.

A singular contribution at $k = \infty$ is needed: $\Lambda_{k_c}(k) = \theta(k_c - k) - k_c\,\delta(k - k_c)$, then $k_c \to \infty$ [12].

$$\langle \mathbf{k}'|\hat{V}_{\text{pp}}|\mathbf{k}\rangle = \frac{g}{L^3}\,\Lambda(k), \qquad \Lambda(k) = 1 - \frac{\delta(1/k)}{k} : \text{ depends on the incoming momentum only.}$$

In practice: $\Lambda = 1$ at finite k, and $\int_0^\infty \Lambda(k)\,\mathrm{d}k = 0$. Form used in the Bogoliubov and BCS Hamiltonians ($L^3 \equiv V$, $\mathbf{k}$ incoming relative momentum). Not Hermitian on the whole Hilbert space; fine on the Bethe–Peierls domain.

Using Λ: the bound state

$E = -|E|$, Fourier transform $\tilde{\psi}(\mathbf{k}) = \int \psi \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \mathrm{d}^3 r$:

$$\left(|E| + \frac{\hbar^2 k^2}{2\mu} \right) \tilde{\psi}(\mathbf{k}) + g\,\mathcal{I} = 0, \qquad \mathcal{I} = L[\psi] = \int \Lambda(k) \tilde{\psi}(\mathbf{k}) \frac{\mathrm{d}^3 k}{(2\pi)^3}.$$

So $\tilde{\psi} = -g\mathcal{I}/(|E| + \hbar^2 k^2/2\mu)$ (i.e. $\psi \propto \mathrm{e}^{-qr}/r$), and self-consistency for $\mathcal{I}$:

$$-\frac{2\pi^2}{g} = \int_0^\infty \frac{\Lambda(k)\, k^2}{|E| + \hbar^2 k^2/(2\mu)} \mathrm{d}k.$$

Divergent if $\Lambda \to 1$. Subtract $\int \Lambda(k) \frac{2\mu}{\hbar^2} \mathrm{d}k = 0$:

$$-\frac{2\pi^2}{g} = -\frac{2\mu|E|}{\hbar^2} \int_0^\infty \frac{\mathrm{d}k}{|E| + \hbar^2 k^2/(2\mu)} = -\frac{\pi}{2} \left(\frac{2\mu}{\hbar^2} \right)^{3/2} \sqrt{|E|}.$$

Possible only for $a > 0$, and gives back $E = -\hbar^2/(2\mu a^2)$.

Using Λ: the Born series

First order: $\mathcal{T}_1(\mathbf{k}', \mathbf{k}) = g\Lambda(k) = g$ (k finite).

Second order: Λ of the intermediate momentum k'', incoming in the second collision:

$$\begin{aligned}\mathcal{T}_2(\mathbf{k}', \mathbf{k}) &= g^2 \int \frac{\Lambda(k'')}{\hbar^2(k^2 - k''^2)/(2\mu) + \mathrm{i}\eta} \frac{\mathrm{d}^3 k''}{(2\pi)^3} \\ &= \frac{g^2}{2\pi^2} \int_0^\infty \Lambda(k'') \left[\frac{k''^2}{\hbar^2(k^2 - k''^2)/(2\mu) + \mathrm{i}\eta} + \frac{2\mu}{\hbar^2} \right] \mathrm{d}k'' \\ &= \frac{g^2 \mu k^2}{\pi^2 \hbar^2} \int_0^\infty \frac{\mathrm{d}k''}{k^2 - k''^2 + \mathrm{i}\eta} = -\mathrm{i}g^2 \frac{\mu k}{2\pi\hbar^2} = -\mathrm{i}gka.\end{aligned}$$

Separable potential: geometric series, $\mathcal{T}_{n+1} = g(-\mathrm{i}ka)^n$, summing to the exact result

$$\mathcal{T}(\mathbf{k}', \mathbf{k}) = \frac{g}{1 + \mathrm{i}ka} = g - \mathrm{i}gka + \ldots$$

The Born approximation violates unitarity: $\mathcal{T}_1 = g$ is real, while the optical theorem requires $\mathrm{Im}\, f(0) = k\sigma/4\pi \neq 0$. Cured at second order: $\mathcal{T}_2$ gives exactly $\mathrm{Im}\, f(0) = ka^2 = k\sigma/(4\pi)$.

Equivalence with a renormalized coupling constant

Common alternative: contact potential $\tilde{V}(\mathbf{k}' - \mathbf{k}) = g_0$ with a cutoff $k, k' < k_c$. Separable: the Born series is geometric,

$$\mathcal{T}(\mathbf{k}', \mathbf{k}) = \frac{g_0}{1 - g_0 \Pi(E)}, \qquad \Pi(E) = \int_{k'' < k_c} \frac{1}{E - \hbar^2 k''^2/(2\mu) + \mathrm{i}\eta} \frac{\mathrm{d}^3 k''}{(2\pi)^3} \quad \text{(linearly divergent)}.$$

Fix g_0 by imposing $\mathcal{T} = g$ at $E = 0$:

$$\frac{1}{g_0} = \frac{1}{g} - \int_{k < k_c} \frac{2\mu}{\hbar^2 k^2} \frac{\mathrm{d}^3 k}{(2\pi)^3} = \frac{\mu}{2\pi\hbar^2 a} - \frac{\mu k_c}{\pi^2 \hbar^2}$$

$g_0 \to 0^-$ as $k_c \to \infty$, whatever the sign of a. Then, at all orders,

$$\frac{1}{\mathcal{T}(\mathbf{k}', \mathbf{k})} = \frac{1}{g} - [\Pi(E) - \Pi(0)] = \frac{1 + \mathrm{i}ka}{g}.$$

Physical results depend on (g_0, k_c) only through a. Same counterterm $\int \mathrm{d}^3 k / k^2$ as the prescription $\int \Lambda \, \mathrm{d}k = 0$.

Summary – Chapter 4 (1/2)

- Two-body problem $\to$ a particle of reduced mass μ in $V(\mathbf{r})$. Scattering is described by the amplitude $f(\mathbf{k}, \mathbf{k}')$, with $\mathrm{d}\sigma/\mathrm{d}\Omega = |f|^2$.
- **Lippmann–Schwinger**: $|\psi_{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \hat{G}_0^{(+)} \hat{V} |\psi_{\mathbf{k}}\rangle$, the $+\mathrm{i}\eta$ selecting outgoing waves; $f = -\frac{\mu}{2\pi\hbar^2} \mathcal{T}(\mathbf{k}', \mathbf{k})$.
- **Born approximation**: $f = -\frac{\mu}{2\pi\hbar^2} \tilde{V}(\mathbf{q})$. Valid at high energy or for weak potentials; recovers Rutherford and Bragg scattering. The Born series fails when V binds.
- **Partial waves**: $S_\ell = \mathrm{e}^{2\mathrm{i}\delta_\ell}$, unitary limit, optical theorem. Bound states are poles of S_ℓ on $\mathrm{i}\mathbb{R}_+$.
- **Low energy**: $\tan\delta_\ell \propto k^{2\ell+1}$, only the s wave survives. $f \simeq -a/(1 + \mathrm{i}ka)$; a weakly bound state $-\hbar^2/(2\mu a^2)$ when $a \gg b > 0$.

Summary – Chapter 4 (2/2)

- **Identical particles**: interference between $f(\mathbf{k}, \mathbf{k}')$ and $f(\mathbf{k}, -\mathbf{k}')$. Even (odd) partial waves only for bosons (fermions): polarized fermions do not interact at low energy.
- **Examples**: hard sphere, $a = R$ and $\sigma = 4\pi R^2$; square well, a diverges each time a bound state appears.
- **Resonances**: bound states, virtual states and quasi-bound states as poles of S_ℓ; Breit–Wigner line shape. Feshbach resonances tune $a(B) = a_{\mathrm{bg}}[1 - \Delta/(B - B_0)]$.
- **Pseudopotential** $g\,\delta(\mathbf{r})\partial_r(r\,\cdot)$ with $g = 2\pi\hbar^2 a/\mu$: exact $f = -a/(1 + \mathrm{i}ka)$. In momentum space $\langle \mathbf{k}'|\hat{V}_{\mathrm{pp}}|\mathbf{k}\rangle = g\Lambda(k)/L^3$, equivalent to a renormalized coupling $1/g_0 = 1/g - \int 2\mu/(\hbar^2 k^2)$. The tool for Bogoliubov and BCS theories.

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