ADVANCED QUANTUM MECHANICS

TUTORIALS 2024–2025

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Please ask me MANY questions!

Wednesday, December 4$^{\text{th}}$, 2024

Outline of the tutorials for the whole semester

- **Problem 1:** two–particle interference
- **Problem 2:** coherence and correlations in quantum gases
- **Problem 3:** lattice models, superfluid/Mott insulator transition
- **Problem 4:** Quantum scattering, scattering resonances

All problems describe experiments that have actually been performed

They all contain elements of theory and introduce calculation techniques

They all contain both standard questions and (very?) hard questions

A bird's eye view of the problem

Problem #4: Quantum scattering and scattering resonances

- Review: scattering problems with optical waves

  Fabry–Pérot interferometer

- Quantum scattering theory

  Partial waves, *s*–wave phase shift, scattering length

- Single–channel scattering resonances: "shape resonances"

  Square well, shape resonances due to the centrifugal barrier

- Scattering resonances involving multiple channels: "Feshbach resonances"

  Two–channel model, experimental applications

Review:

A scattering problem with optical waves

The Fabry–Pérot interferometer

This example has a direct connection to quantum 'shape resonances'

[Hecht, *Optics*, 5$^{\text{th}}$ edition, Pearson (2017), §9.6]

Electromagnetic wave propagating in 1D (qu. 1)

- The propagation equation for an electromagnetic wave in vacuum $(\nabla \cdot \mathbf{E} = 0)$

  follows from Maxwell's equations $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t$ and $\nabla \times \mathbf{B} = \frac{1}{c^2}\,\partial \mathbf{E}/\partial t$

  The identity $\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E}$ yields: $\nabla^2 \mathbf{E} - \frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} = \mathbf{0}$

- Monochromatic wave: single frequency ω $\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})\,\exp(-i\omega t)$

  The propagation equation reduces to: $-\nabla^2 \mathbf{E} = \frac{\omega^2}{c^2}\,\mathbf{E}$

  Plane–wave solutions $\mathscr{E}\mathbf{e}\exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]$ satisfy $k = \omega/c$

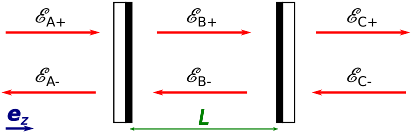
  All solutions $\mathbf{E}(z,t)$ propagating along z are linear combinations of plane waves:

$$\mathbf{E} = \mathscr{E}_+\mathbf{e}_+\exp\left[i(kz - \omega t)\right] + \mathscr{E}_-\mathbf{e}_-\exp\left[i(-kz - \omega t)\right]$$

- Due to Gauss's flux theorem $\nabla \cdot \mathbf{E} = 0$,

  the polarisations $\mathbf{e}_+$ and $\mathbf{e}_-$ are both perpendicular to $\mathbf{k} = k\,\mathbf{e}_z$

Electromagnetic wave and Fabry–Pérot cavity (qu. 2)



- Two parallel semi–reflecting mirrors

  (amplitude) transmission & reflection coefficients:

  t and r (both assumed to be real)

- Propagation perpendicular to mirrors: $\mathbf{k} = k\mathbf{e}_z$

  Assume a single polarisation is present: $\mathbf{E} = \mathbf{e}\,\mathscr{E}(\mathbf{r},t)$

- Monochromatic solution of the propagation equation: $\mathbf{E}(z,t) = \mathbf{E}(z)\,\exp(-i\omega t)$

  Analogue of the condition for a stationary state in quantum mechanics

- Three spatial regions: A (left), B (cavity = between the mirrors), C (right)

  In each region α, the electric field is a sum of two counterpropagating plane waves:

$$\mathbf{E}(z,t) = \mathbf{e}\left[\mathscr{E}_{\alpha+}\exp(ikz) + \mathscr{E}_{\alpha-}\exp(-ikz)\right]\exp(-i\omega t)$$

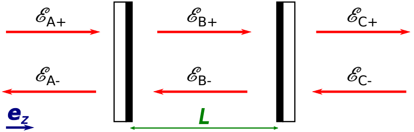
- Propagation equation is 2nd–order: $\dfrac{d^2\mathbf{E}}{dz^2} = \dfrac{\omega^2}{c^2}\mathbf{E}$ so 2 conditions are required

  For an ‘initial value problem’, we would give $\mathscr{E}_{A+}$ and $\mathscr{E}_{A-}$ **NOT TODAY!**

  Scattering problem: impose $\mathscr{E}_{C-} = 0$

  The solution is proportional to the incident flux $\mathscr{E}_{A+}$: choose $\mathscr{E}_{A+} = \mathscr{E}_I$

Fabry–Pérot: transmission/reflection coefficients (qu. 3)



Scattering problem: $\mathcal{E}_{C-} = 0$ and $\mathcal{E}_{A+} = \mathcal{E}_I$

- Write the transmission and reflection coefficients in matrix form at both mirrors

  The two mirrors are identical, but **beware:** their two sides are not symmetric!

The minus sign comes from the unitarity of U: it enforces conservation of energy at each mirror

Beware: also account for propagation between the mirrors: phases $\exp(\pm ikL)$

$$\begin{pmatrix} \mathcal{E}_{B+} \\ \mathcal{E}_{A-} \end{pmatrix} = \begin{pmatrix} t & -r \\ r & t \end{pmatrix} \begin{pmatrix} \mathcal{E}_{A+} \\ \mathcal{E}_{B-} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathcal{E}_{B-}\, e^{-ikL} \\ \mathcal{E}_{C+}\, e^{+ikL} \end{pmatrix} = \begin{pmatrix} t & -r \\ r & t \end{pmatrix} \begin{pmatrix} \mathcal{E}_{C-}\, e^{-ikL} \\ \mathcal{E}_{B+}\, e^{+ikL} \end{pmatrix}$$

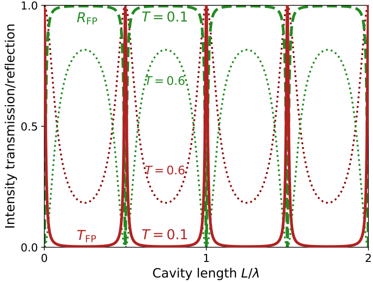
- Transmission and reflection coefficients for the Fabry–Pérot (FP) cavity:

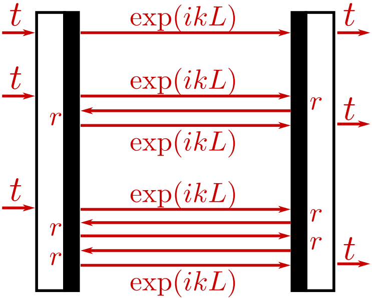
$$t_{\text{FP}} = \frac{\mathcal{E}_{C+}\exp(ikL)}{\mathcal{E}_{A+}} = \frac{t^2\exp(ikL)}{1 - r^2\exp(2ikL)} \quad \text{and} \quad r_{\text{FP}} = \frac{\mathcal{E}_{A-}}{\mathcal{E}_{A+}} = r\,\frac{1-\exp(2ikL)}{1 - r^2\exp(2ikL)}$$

Fabry–Pérot: resonant cavity (qu. 4)

$$t_{\mathrm{FP}} = \frac{t^2 \exp(ikL)}{1 - r^2 \exp(2ikL)} \quad \text{and} \quad r_{\mathrm{FP}} = r\,\frac{1 - \exp(2ikL)}{1 - r^2 \exp(2ikL)}, \qquad T_{\mathrm{FP}} = |t_{\mathrm{FP}}|^2 \quad \text{and} \quad R_{\mathrm{FP}} = |r_{\mathrm{FP}}|^2$$

- If $2L$ is an integer multiple of λ, $2L = p\lambda$,
  Perfect transmission: $t_{\mathrm{FP}} = (-1)^p$, $r_{\mathrm{FP}} = 0$
  independent of the transmission of a single mirror
  Smaller t leads to better selectivity





$$t_{\mathrm{FP}} = t\,e^{ikL}\left(1 + (r\,e^{ikL})^2 + (r\,e^{ikL})^4 + \cdots\right) t$$

- The double–transmitted waves all interfere: multiple–wave interference
- Constructive interference
  if all double–transmitted waves are in phase,
  that is, if $2kL = p\,2\pi$

Quantum scattering

1. *s*–wave scattering; scattering resonances

2. Partial–wave expansion

3. Zero–range potential

[Bloch, Dalibard, Zwerger, Rev. Mod. Phys. **80**, 885 (2008), §I]
[Messiah, *Quantum Mechanics*, volume II, Wiley (1966), chap. XIX]

The scattering state: a *stationary* quantum state (qu. 5)

- **Two particles collide in free space:** no trap, centre–of–mass referential

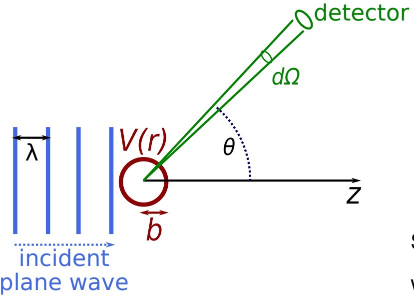
For $r \to \infty$, the interaction potential $V(\mathbf{r})$ is negligible compared to the kinetic energy

Compare it to $\hbar^2/(mr^2)$: For van der Waals interactions $V_{\rm vdw}(r) = C_6/r^6$, $b = l_{\rm vdw} = (mC_6/\hbar^2)^{1/4}$

DOES NOT APPLY to Coulomb interaction [see also Problem 2, slide 21/75]

- We impose a **boundary condition for large** r ($r \gg b$, range of the interaction)

$$\Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\Omega)\,\frac{e^{ikr}}{r}$$



The length $f_{\mathbf{k}}(\Omega)$ is the scattering amplitude, to be determined by solving Schrödinger Eq.

- Unlike for bound states, the energy is known before calculating $|\Psi\rangle$: $E = \hbar^2k^2/(2m)$
- **This is not an initial value problem!**

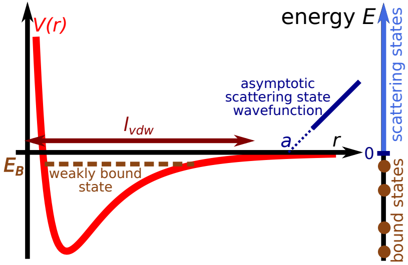
Solve $H|\Psi\rangle = \dfrac{\hbar^2k^2}{2m}|\Psi\rangle$ to find $f_{\mathbf{k}}(\Omega)$,

which generalises t and r

Scattering cross section in solid angle Ω: $\dfrac{d\sigma}{d\Omega} = |f_{\mathbf{k}}(\Omega)|^2$

Bound states and scattering states: normalisation (qu. 6)

$$H = \frac{\mathbf{p}^2}{2m} + V(r), \qquad \Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\Omega)\, e^{ikr}/r$$



- The potential $V(r)$ describing the interaction between 2 particles reaches an asymptote for $r \to \infty$: choose it as the energy $E = 0$
- Scattering states for 2 momenta $\mathbf{k}_1 \neq \mathbf{k}_2$ are orthogonal: $\langle \Psi_{\mathbf{k}_1} | \Psi_{\mathbf{k}_2} \rangle = 0$ (easy if $|k_1| \neq |k_2|$, harder if $|k_1| = |k_2|$)

- Eigenstates $|\Psi_n\rangle$ of H with $E < 0$ are bound states: $\langle \mathbf{r} | \Psi_n \rangle$ goes to 0 for $r \to \infty$

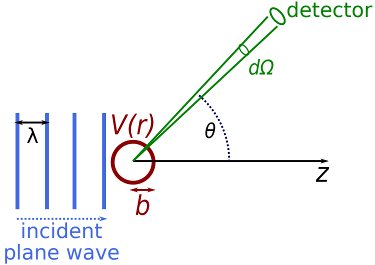
  Labelled by a discrete index n, $\displaystyle\int d^3r\, |\psi_n|^2 = 1$,

- Eigenstates $|\Psi_{\mathbf{k}}\rangle$ of H with $E \geq 0$ are scattering states:

  Labelled by the wavevector $\mathbf{k}$ such that $E = \hbar^2\mathbf{k}^2/(2m)$: continuous set of values

  $\langle \mathbf{r} | \Psi_{\mathbf{k}} \rangle$ DOES NOT go to zero for $r \to \infty$, so $|\Psi_{\mathbf{k}}\rangle$ cannot be normalised to 1

Normalisation for a scattering state (qu. 6)



$$\Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} 1 \times e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\Omega)\, \frac{e^{ikr}}{r}$$

- Choose the coefficient 1 in front of the incident plane wave

  namely: choose the amplitude of the incident current $\mathbf{j}_{\mathrm{inc}}$

- Schrödinger current for the incident plane wave $\Psi_{\mathrm{inc}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$:

$$\mathbf{j}_{\mathrm{inc}}(\mathbf{r}) = \frac{\hbar}{2mi}\left(\Psi^*_{\mathrm{inc}}\nabla\Psi_{\mathrm{inc}} - \Psi_{\mathrm{inc}}\nabla\Psi^*_{\mathrm{inc}}\right) = \frac{\hbar\mathbf{k}}{m} = v\,\mathbf{e}_z$$

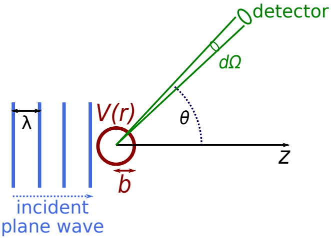
  Therefore, the incident flux $\mathbf{j}_{\mathrm{inc}} \cdot dS\,\mathbf{e}_z$ on the elementary surface $dS\,e_{\mathbf{z}}$ is $v\,dS$

- The scattering state $|\Psi_{\mathbf{k}}\rangle$ and amplitude $f_{\mathbf{k}}(\Omega)$ are fully determined by this choice

  Just like in 1D, where t and r are defined for the incident plane wave e^{ikz}

Zero–energy scattering state, **scattering length** (qu. 7, 8)

- From now on, we assume that the interaction $V(r)$ is *spherically symmetric*
  (this excludes anisotropic dipole–dipole interaction)



$$\Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\Omega)\,\frac{e^{ikr}}{r}$$

- For $E > 0$, the wavevector $\mathbf{k} \neq \mathbf{0}$

the scattering state $\Psi_{\mathbf{k}}$ is **not** spherically–symmetric
cylindrical symmetry about the incidence direction $\mathbf{k}$

- For $E = 0$, the incident wavevector $\mathbf{k} = 0$, and the scattering amplitude $f_{\mathbf{0}} = -a$

  The scattering state is spherically symmetric: $\Psi_{\mathbf{0}}(r) \underset{r\to\infty}{=} 1 - \frac{a}{r}$

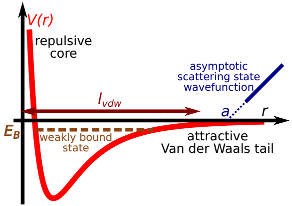
- **In a dilute system,** (i.e. holds in a gas)

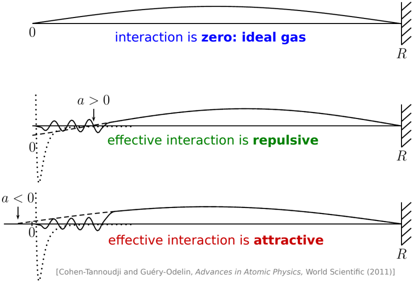
  the **scattering length** a encodes all properties of low–energy scattering

Related to s–wave **phase shift** δ_0 in partial wave expansion: $f_l = (e^{2i\delta_l} - 1)/(2ik)$ and $\delta_0 = -ka$

Universal scattering at low energy, effective interaction

- **2–body problem:** for $r > b$, behaviour of low–energy wavefunctions is piloted by a

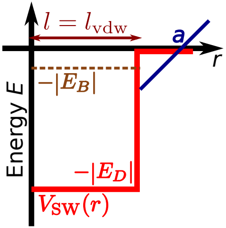




[Cohen-Tannoudji and Guéry-Odelin, *Advances in Atomic Physics*, World Scientific (2011)]

- The mean distance between atoms is $n^{-1/3} = (L^3/N)^{1/3}$

Dilute system: If $n^{-1/3}$ is larger than the interaction range b, the short–range details of the potential are irrelevant
All potentials with the same scattering length are equivalent



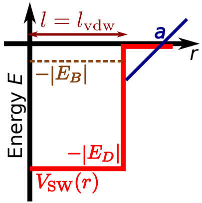
- Replace the potential

by a simpler one with the same scattering length:
square well or **contact potential** "$g\,\delta(\mathbf{r})$" with $g = 4\pi\hbar^2 a/m$

Beware: contact potentials must be handled with care! (details soon)

Scattering length for a square well (1/2) (qu. 15)

$$H = \mathbf{p}^2/(2m) + V(r), \qquad \Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\Omega)\, e^{ikr}/r$$



- 3D isotropic square well potential $V_{\mathrm{SW}}(r)$:
  $V_{\mathrm{SW}}(r) = -|E_D|$ for $r \leq l$ and $V_{\mathrm{SW}}(r) = 0$ for $r > l$
- Calculate zero–energy scattering state $\Psi_0(r) \underset{r\to\infty}{=} 1 - a/r$
  where the unknown is the scattering length a

- The potential $V_{\mathrm{SW}}(r)$ and boundary condition are both spherically symmetric therefore, look for a spherically–symmetric wavefunction $\Psi_0(r)$

- For $r > 0$, Laplacian of a spherically–symmetric function: $\nabla^2\Psi_0(r) = \frac{1}{r}\frac{d^2}{dr^2}(r\,\Psi_0)$

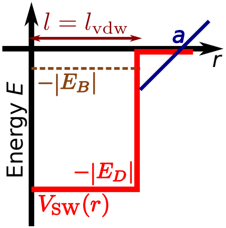
  Zero–energy Schrödinger equation: $0 = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(r\Psi_0) + V_{\mathrm{SW}}(r)\,(r\Psi_0)$

  The 3D Schrödinger Eq. reduces to a 1D Schrödinger Eq. on $u_0(r) = r\,\Psi_0(r)$

- Boundary condition *(a)*: For large r, $u_0(r) \underset{r\to\infty}{=} r - a$ is linear in r

  Boundary condition *(b)*: For $r \to 0$, $\Psi_0(0)$ is finite, therefore $u_0(0) = 0 \times \Psi_0(0) = 0$

Scattering length for a square well (2/2) (qu. 15)



- Spherically–symmetric square well potential $V_{\rm SW}(r)$:

$$V_{\rm SW}(r) = -|E_D| = -\frac{\hbar^2 k_D^2}{2m} \quad \text{for } r \le l \quad \text{and} \quad V_{\rm SW}(r) = 0 \text{ for } r > l$$

- Schrödinger equation: $$0 = -\frac{\hbar^2}{2m} u_0''(r) + V_{\rm SW}(r)\, u_0(r)$$
- Boundary conditions: $u_0(0) = 0$ and $u_0(r) \underset{r\to\infty}{=} r - a$

  where the unknown is the scattering length a

(a) For $r > l$: $V_{\rm SW}(r) = 0$, so that $u_0''(r) = 0$, thus $u_0(r) = r - a$

(b) For $r < l$: $V_{\rm SW}(r) = -\frac{\hbar^2 k_D^2}{2m}$, so that $u_0''(r) + k_D^2\, u_0(r) = 0$, thus $u_0(r) = \alpha \sin(k_D\, r)$

- Matching condition: $u_0'(r)/u_0(r)$ must be continuous at $r = l$

$$\frac{1}{l-a} = \frac{k_D \cos(k_D l)}{\sin(k_D l)}, \qquad \text{therefore} \qquad \frac{a}{l} = 1 - \frac{\tan(k_D l)}{k_D l}$$

Scattering resonance for all $k_D l = (n + 1/2)\,\pi$, where n is an integer

that it to say, for all well depths $|E_D| = (n+1/2)^2\, \pi^2\, \frac{\hbar^2}{2ml^2}$

s–wave bound states for a square well (1/2) (qu. 16)

$V_{\rm SW}(r) = -|E_D|$ for $r \le l$ and $V_{\rm SW}(r) = 0$ for $r > l$; $|E_D| = \hbar^2 k_D^2/(2m)$

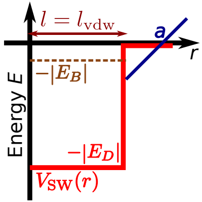
- $H = \dfrac{\mathbf{p}^2}{2m} + V(r)$ commutes with $\mathbf{l}$: look for eigenstates $|\Psi_{n,l,m}\rangle$ shared by H, $\mathbf{l}^2$, l_z

  $l^2\,|\Psi_{n,l,m}\rangle = \hbar^2 l(l+1)\,|\Psi_{n,l,m}\rangle$ and $l_z\,|\Psi_{n,l,m}\rangle = \hbar\, m\,|\Psi_{n,l,m}\rangle$

- s–wave bound states: $l = m = 0$ energy $-|E_D| \le E_n = -\hbar^2\kappa_n^2/(2m) < 0$

  $\psi_{n,0,0}(r)$ depends only on $r = |\mathbf{r}|$: write $\psi_{n,0,0}(r) = u_n(r)/r$ with $u_n(0) = 0$

$$-\frac{\hbar^2}{2m}\,u_n''(r) + V_{\rm SW}(r)\,u_n(r) = -\frac{\hbar^2\kappa_n^2}{2m}\,u_n(r)$$



- For $r > l$, $u_n''(r) = \kappa_n^2\,u_n(r)$ so that $u_n(r) = \alpha\, e^{-\kappa_n r}$

  ($e^{+\kappa_n r}$ would lead to a wavefunction which is not normalisable)

- For $r < l$, $-\dfrac{\hbar^2}{2m}\,u_n''(r) - \dfrac{\hbar^2 k_D^2}{2m}\,u_n(r) = -\dfrac{\hbar^2\kappa_n^2}{2m}\,u_n(r)$

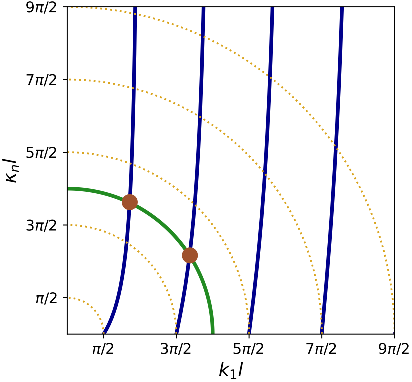
  $u_n''(r) + k_1^2 u_n(r) = 0$ with $k_1^2 = k_D^2 - \kappa_n^2 \ge 0$

  Using $u_n(0) = 0$, $u_n(r) = \beta\sin(k_1 r)$

- Matching condition: $\dfrac{u_n'(r)}{u_n(r)}$ is continuous at $r = l$, hence $-\kappa_n\, l = \dfrac{k_1\, l}{\tan(k_1\, l)}$

s–wave bound states for a square well (2/2) (qu. 17)

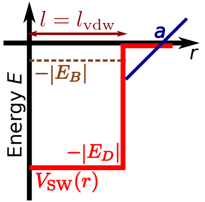
Bound–state energies: $\dfrac{E_n}{\hbar^2/(2ml^2)} = -(\kappa_n l)^2$ with $\kappa_n l = -\dfrac{k_1 l}{\tan(k_1 l)} > 0$ and $(k_D l)^2 = (k_1 l)^2 + (\kappa l)^2$



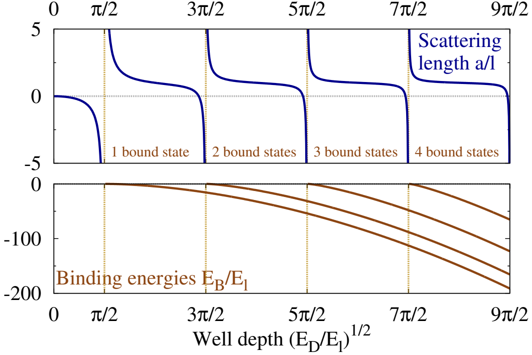
- Graphical solution: look for the intersections of the blue and green curves in the $(k_1 l, \kappa_n l)$ quarter–plane $(k_1 > 0,\ \kappa_n > 0)$
- If $(n - 1/2)\,\pi < k_D\,l < (n + 1/2)\,\pi$, n intersections, hence, n bound states
  $n = 2$ on the figure

- For every $k_D l = (n + 1/2)\,\pi$, a new bound state appears
  correspondingly, the scattering length a/l diverges

Square well: zero–energy scattering resonance (qu. 18, 19)



Unit of energy: $E_l = \hbar^2/(2ml^2)$



- The scattering length diverges every time a new bound state enters the well
- The new bound state appears with the energy $E = 0$: zero–energy resonance

  The square well plays the role of the Fabry–Perot cavity

  The analogy has limitations: the spatial extent of the bound state is $a \gg l$

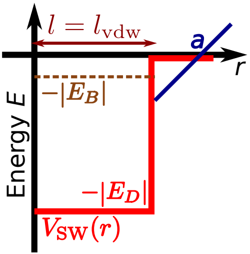
- This is a general property known as LEVINSON'S theorem:

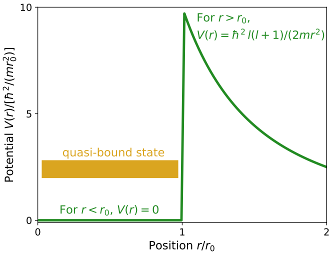
  For any spherically–symmetric potential $V(r)$ (smooth and well–behaved for $r \to 0$ and $r \to +\infty$), the scattering length a diverges each time a new bound state appears

  [C. Cohen–Tannoudji & D. Guéry–Odelin, *Advances in Atomic Physics*, World Scientific (2011), Sec. 15.3.3]

Fabry–Pérot analogue: scattering resonance

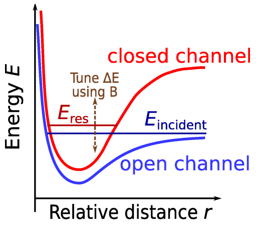
- Simplest example: one scattering channel **'shape resonance'**

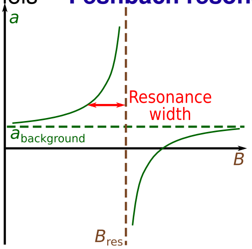




[Messiah, *Quantum Mechanics*, Wiley (1958), vol. I, chapter 10, §15]

- More useful experimentally: two coupled channels **Feshbach resonance**





[Bloch, Dalibard, Zwerger, Rev. Mod. Phys. **80**, 885 (2008), §I.C]

Dilute system: from 2–body to many–body physics

We assume that the system is **dilute:** $n^{-1/3} \gg b$ (interaction range)

- **2–body physics:** for a given potential $V(r)$, determine the scattering length a
  Choose the correct **effective contact interaction** "$g\,\delta(\mathbf{r})$" with $g = 4\pi\hbar^2 a/m$

- **Many–body physics:** work with the contact interaction term $g\,\hat{\Psi}^\dagger\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}$
  For weakly–interacting bosons at zero temperature, often reduces to Gross–Pitaevskii Eq.
  Fermions are more complicated (BEC–BCS crossover . . .)

- **Beware:** the system may be **both** dilute **and** strongly interacting

$$b \ll n^{-1/3} \lesssim a$$

This regime is called 'resonant', or 'strongly correlated', or 'unitary'
It is accessible experimentally with fermions, currently explored with bosons
Mean–field theory is not applicable, but many surprising symmetries

[Castin & Werner, in *The BCS–BEC crossover and the unitary Fermi gas*, Lecture Notes in Physics **836**, Zwerger (ed), Springer (2012)]

Tuning the interaction between many bosonic atoms

- Simplest many–body description: **Gross–Pitaevskii equation (GPE)**

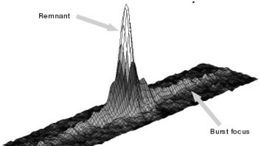
  This is a mean–field theory, valid at zero temperature $T = 0$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + U_{\text{trap}}(\mathbf{r}) \Psi + g |\Psi(\mathbf{r})|^2 \Psi$$

"Attractive" $a<0$ BEC collapses

"Ideal Gas" $a=0$

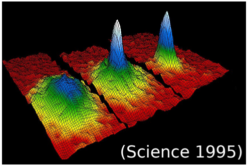
"Repulsive" $a>0$ BEC is stable



(Nature 2001)

Cornell & Wieman

^{85}Rb



(Science 1995)

For $a < 0$ and many atoms, the later stages of the collapse are not captured by Gross–Pitaevskii Eq.

[Pitaevskii & Stringari, *Bose–Einstein Condensation & Superfluidity*, OUP (2016), §5.1, §11.2, §11.6]

Tuning the interaction between many fermionic atoms

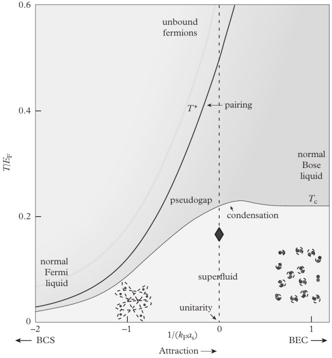
- In order to beat Pauli's exclusion, we need at least
  2 different species (e.g. $^{6}\mathrm{Li}$, $^{40}\mathrm{K}$) or 2 internal states of the same atom ($|\uparrow\rangle$, $|\downarrow\rangle$)

- For fermions, **there is no Gross–Pitaevskii equation**

Long–range order on 2–atom correlator: $|F(\mathbf{r}_1,\mathbf{r}_2)|^2 = \lim_{r\to\infty} \langle \hat{\Psi}^\dagger_\uparrow(\mathbf{r}_2+\mathbf{r})\hat{\Psi}^\dagger_\downarrow(\mathbf{r}_1+\mathbf{r})\hat{\Psi}_\downarrow(\mathbf{r}_1)\hat{\Psi}_\uparrow(\mathbf{r}_2)\rangle$

Mean–field description through the Bogoliubov–de Gennes equations

For more details, solve the **Homework problem**



[Sá de Melo, Physics Today **61**(10), 45 (2018)]

Scattering by a spherically–symmetric potential:

Partial–wave expansion

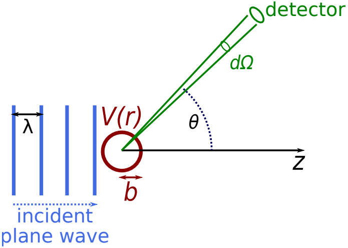
[Messiah, *Quantum Mechanics,* Wiley (1958), vol. I, §X.8 & §X.11–15; vol. II, exercice XIX.4]

Scattering state $|\Psi_{\mathbf{k}}\rangle$ in terms of spherical harmonics (9)

- The spherical harmonics $Y_{l,m}(\hat{\mathbf{r}}) = Y_{l,m}(\Omega) = Y_{l,m}(\theta,\phi)$ ($\hat{\mathbf{r}}$ = vector of unit length) make up a basis of the (square–integrable) functions on the sphere

  Therefore, for a given r, we may expand $\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} \Psi_{\mathbf{k},l,m}(r)\, Y_{l,m}(\hat{\mathbf{r}})$

  where the 'coefficients' $\Psi_{\mathbf{k},l,m}(r)$ depend on $r = |\mathbf{r}|$ only



- The scattering state $|\Psi_{\mathbf{k}}\rangle$ is cylindrically–symmetric about the incident direction $\mathbf{k} = k\,\mathbf{e}_z$: no dependence on the azimuthal angle ϕ
- The dependence on ϕ of $Y_{l,m}(\mathbf{r})$ is $e^{im\phi}$ Hence, keep only $m = 0$ in the sum

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{+\infty} \Psi_{k,l}(r)\, Y_{l,0}(\hat{\mathbf{r}})$$

($\mathbf{k} = k\mathbf{e}_z$, hence, the subscript k in $\Psi_{k,l}$ is no longer a vector)

- Each term in the sum is an eigenstate of both $\mathbf{l}^2$ and l_z (neither of which involves r)

$$\mathbf{l}^2\,|Y_{l,m}\rangle = \hbar^2 l(l+1)\,|Y_{l,m}\rangle \quad \text{and} \quad l_z\,|Y_{l,m}\rangle = \hbar m\,|Y_{l,m}\rangle$$

[Kosmann–Schwarzbach, *Groups and Symmetries*, Springer (2010), chap. 7]

Schrödinger Eq. on the l^{th} component $\Psi_{\mathbf{k},l}(r)$ (qu. 10)

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{+\infty} \Psi_{k,l}(r)\, Y_{l,0}(\hat{\mathbf{r}}), \quad \mathbf{l}^2\,|Y_{l,m}\rangle = \hbar^2 l(l+1)\,|Y_{l,m}\rangle, \quad l_z\,|Y_{l,m}\rangle = \hbar m\,|Y_{l,m}\rangle, \quad E = \frac{\hbar^2 k^2}{2m}$$

- Schrödinger equation on the full scattering state $|\Psi_{\mathbf{k}}\rangle$:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_{\mathbf{k}} \;+\; V(r)\,\Psi_{\mathbf{k}} \;=\; \frac{\hbar^2 k^2}{2m}\,\Psi_{\mathbf{k}}$$

- Laplacian acting on a function expressed in spherical coordinates $f(r,\theta,\phi)$:

$$\nabla^2 f \;=\; \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,f) \;-\; \frac{\mathbf{l}^2/\hbar^2}{r^2}\,f \qquad \text{where } \mathbf{l}^2 = \text{squared angular momentum operator}$$

- $\nabla^2\left[\Psi_{k,l}(r)\,Y_{l,0}(\hat{\mathbf{r}})\right] = \left[\frac{1}{r}\frac{\partial}{\partial r^2}(r\,\psi_{k,l}) - \frac{l(l+1)}{r^2}\,\psi_{k,l}\right] Y_{l,0}(\hat{\mathbf{r}})$ proportional to $|Y_{l,0}\rangle$

  The spherical harmonics $|Y_{l,0}\rangle$ are linearly independent

- This leads to a Schrödinger Eq. for each component $\Psi_{k,l}$ with quantum number l:

$$-\frac{\hbar^2}{2m}\,\frac{1}{r}\,\frac{\partial^2(r\Psi_{k,l})}{\partial r^2} \;+\; \left(\frac{\hbar^2}{2m}\,\frac{l(l+1)}{r^2} + V(r)\right)\Psi_{k,l} \;=\; \frac{\hbar^2 k^2}{2m}\,\Psi_{k,l}$$

  The angular part of the Laplacian yields the centrifugal barrier $l(l+1)/r^2$

Boundary conditions on the partial wave $|\Psi_{k,l}\rangle$ (qu. 11)

Previous formulation of the scattering problem: (not an initial value problem)

$$H\,|\Psi_{\mathbf{k}}\rangle = \frac{\hbar^2 k^2}{2m}\,|\Psi_{\mathbf{k}}\rangle \quad \text{with} \quad \Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} e^{i\,\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k},\hat{\mathbf{r}})\,\frac{e^{ikr}}{r}$$

- Assuming that $V(r)$ is spherically symmetric, we have replaced the partial differential equation involving a complicated boundary condition by **uncoupled ordinary differential equations**, labelled by the integer l

$$-\frac{\hbar^2}{2m}\,\frac{d^2(r\,\Psi_{k,l})}{dr^2} + \left(\frac{\hbar^2}{2m}\,\frac{l(l+1)}{r^2} + V(r)\right)(r\,\Psi_{k,l}) = \frac{\hbar^2\,k^2}{2m}\,(r\,\Psi_{k,l})$$

- $\Psi_{k,l}(r)$ is finite for $r \to 0$, therefore $u_{k,l}(r) = r\,\Psi_{k,l}(r)$ satisfies $u_{k,l}(0) = 0$

The differential Eq. is 2^{nd}–order: this defines $\Psi_{k,l}(r)$ up to a multiplicative constant α_l

- For large r, both $V(r)$ and $l(l+1)/r^2$ are negligible
  $u''_{k,l}(r) + k^2 u_{k,l} = 0$, meaning that $\Psi_{k,l} = \dfrac{u_{k,l}(r)}{r} \underset{r\to\infty}{=} \alpha_l\,\dfrac{\sin(kr - l\pi/2 + \delta_l)}{r}$

  The phase δ_l is already fully determined. $\alpha_l^{\text{text}} = \alpha_l^{\text{slides}}\,[(2l+1)/(4\pi)]^{1/2}$

- Choose α_l such that the complete wavefunction $\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_l \Psi_{k,l}(r)\,Y_{l,0}(\hat{\mathbf{r}})$ satisfies the scattering boundary condition: $\Psi_{\mathbf{k}}(\mathbf{r}) - e^{i\,\mathbf{k}\cdot\mathbf{r}} \underset{r\to\infty}{=}$ outgoing wave

Expanding a plane wave into l–wave components (1/3)

- The plane wave $\Phi_{\mathbf{k}}(\mathbf{r}) = e^{ikz}$ has a well–defined momentum: $\mathbf{p}\,|\Phi_{\mathbf{k}}\rangle = \hbar k\,\mathbf{e}_z\,|\Phi_{\mathbf{k}}\rangle$
  We shall expand it into components with well–defined angular momentum $\mathbf{l}^2$, l_z

$$\Phi_{\mathbf{k}}(\mathbf{r}) \quad = \quad \sqrt{4\pi}\sum_l (2l+1)^{1/2}\, i^l\, j_l(kr)\, Y_{l,0}(\hat{\mathbf{r}}) \quad = \quad \sum_l (2l+1)\, i^l\, j_l(kr)\, P_l(\cos\theta)$$

SPECIAL FUNCTIONS FREQUENTLY USED IN QUANTUM SCATTERING THEORY:

- **Spherical harmonics** $Y_{l,m}(\hat{r})$ satisfy $\mathbf{l}^2\, Y_{l,m}(\hat{\mathbf{r}}) = \hbar^2 l(l+1)\, Y_{l,m}(\hat{\mathbf{r}})$, $\quad l_z\, Y_{l,m}(\hat{\mathbf{r}}) = \hbar m\, Y_{l,m}(\hat{\mathbf{r}})$

- **Legendre polynomials**

$$P_l(u) \;=\; \frac{1}{2^l\, l!}\left(\frac{d}{dx}\right)^l \left(u^2-1\right)^l$$

  They determine the angular dependence of $Y_{l,0}$:

$$Y_{l,0}(\hat{\mathbf{r}}) \;=\; \left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\cos\theta)$$

- **Spherical Bessel functions** $j_l(\rho)$ [also $y_l(\rho)$]: defined on the next slide

[NIST Dynamical Library of Mathematical Functions, https://dlmf.nist.gov]

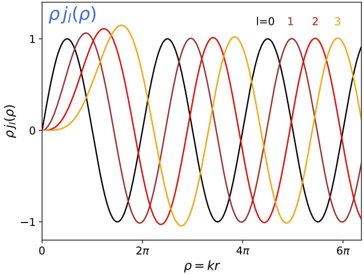
Expanding a plane wave into l–wave components (2/3)

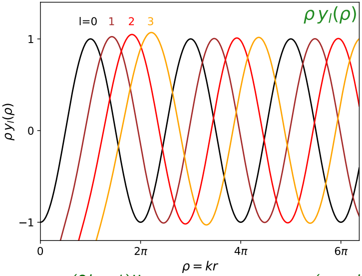
- $\Phi_\mathbf{k}(\mathbf{r}) = e^{ikz} = \sum_l \Phi_{k,l}(r)\, Y_{l,0}(\hat{\mathbf{r}})$ is a solution of $\nabla^2 \Phi_\mathbf{k} = -k^2 \Phi_\mathbf{k}$, so that the $\Phi_{k,l}$ satisfy:

$$-\frac{d^2(r\,\Phi_{k,l})}{dr^2} + \frac{l(l+1)}{r^2}(r\,\Phi_{k,l}) = k^2(r\,\Phi_{k,l}) \qquad \text{[Schrödinger Eq. without } V(r)\text{]}$$

Change variable to $\rho = kr$: $$-\frac{d^2}{d\rho^2}(\rho\,\Phi_l) + \frac{l(l+1)}{\rho^2}(\rho\,\Phi_l) = \rho\,\Phi_l$$

Two independent solutions: the **spherical Bessel functions** $j_l(\rho)$ and $y_l(\rho)$





$$j_l(\rho) \underset{\rho\to 0}{=} \frac{\rho^l}{(2l+1)!!}, \quad j_l(\rho) \underset{\rho\to\infty}{=} \frac{\sin(\rho - l\pi/2)}{\rho} \qquad y_l(\rho) \underset{\rho\to 0}{=} -\frac{(2l-1)!!}{\rho^{l+1}}, \quad y_l(\rho) \underset{\rho\to\infty}{=} -\frac{\cos(\rho - l\pi/2)}{\rho}$$

$(2l)!! = 2l \times (2l-2) \times \cdots \times 2$, $(2l+1)!! = (2l+1) \times (2l-1) \times \cdots \times 1$, $1!! = 0!! = (-1)!! = 1$

- $\Phi_{k,l}$ must be finite for $r \to 0$, therefore $\Phi_{k,l}(r) = \alpha_l\, j_l(r)$

Expanding a plane wave into l–wave components (3/3)

- We have shown $e^{ikz} = \sum_l \alpha_l \, j_l(kr) \, Y_{l,0}(\hat{\mathbf{r}}) = \sum_l \alpha_l \left(\frac{2l+1}{4\pi} \right)^{1/2} j_l(kr) \, P_l(\cos\theta)$

Now, let us determine the coefficients α_l

1. Write the **lowest–order** term in $j_l(\rho)$ as: $j_l(\rho) \underset{\rho \to 0}{=} \frac{2^l \, l!}{(2l+1)!}$

2. Using the explicit formula $P_l(u) = \frac{1}{2^l \, l!} \left(\frac{d}{dx} \right)^l \left(u^2 - 1 \right)^l$,

show that the **highest–order** term in $P_l(u)$ is: $\frac{(2l)!}{2^l \, l! \, l!} \, u^l$

3. Expand both the left– and right–hand sides in increasing powers of $(kr \cos\theta)$

and conclude that $\alpha_l = \left(\frac{4\pi}{2l+1} \right)^{1/2} (2l+1) \, i^l$

$$\Phi_{\mathbf{k}}(\mathbf{r}) = \sqrt{4\pi} \sum_l (2l+1)^{1/2} \, i^l \, j_l(kr) \, Y_{l,0}(\hat{\mathbf{r}}) = \sum_l (2l+1) \, i^l \, j_l(kr) \, P_l(\cos\theta)$$

Scattering state $|\Psi_{\mathbf{k}}\rangle$: scattering amplitude $f_{\mathbf{k}}(\Omega)$ (qu. 12)

- The scattering–state boundary condition $\Psi_{\mathbf{k}}(\mathbf{r}) - \Phi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} f_{\mathbf{k}}(\hat{\mathbf{r}}) \dfrac{e^{ikr}}{r}$

  states that, for large r, the difference $(|\Psi_{\mathbf{k}}\rangle - |\Phi_{\mathbf{k}}\rangle)$ reduces to an outgoing wave

- $$\Phi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} \sum_l \sqrt{4\pi}\,(2l+1)^{1/2}\, i^l \quad \frac{\sin(kr - l\pi/2 \qquad)}{kr} \; Y_{l0}(\hat{\mathbf{r}})$$

  $$\Psi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} \sum_l \sqrt{4\pi}\,(2l+1)^{1/2}\, i^l \;\widetilde{\alpha}_l\; \frac{\sin(kr - l\pi/2 + \delta_l)}{kr} \; Y_{l0}(\hat{\mathbf{r}})$$

  $$(\alpha_l^{\text{slides}} = \sqrt{4\pi}\,(2l+1)^{1/2}\, i^l\, \widetilde{\alpha}_l / k)$$

$$\Psi_{\mathbf{k}}(\mathbf{r}) - \Phi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} \sum_l \frac{[4\pi(2l+1)]^{1/2}}{2ikr} \left[(\widetilde{\alpha}_l e^{i\delta_l} - 1)\, e^{ikr} + (-)^l (-\widetilde{\alpha}_l e^{-i\delta_l} + 1)\, e^{-ikr} \right] Y_{l,0}(\hat{\mathbf{r}})$$

- In order to remove the ingoing wave, choose $\widetilde{\alpha}_l = e^{i\delta_l}$

  $$\Psi_{\mathbf{k}}(\mathbf{r}) - \Phi_{\mathbf{k}}(\mathbf{r}) \underset{r\to\infty}{=} \left(\sum_l [4\pi(2l+1)]^{1/2} \frac{e^{2i\delta_l} - 1}{2ik} Y_{l,0}(\hat{\mathbf{r}}) \right) \frac{e^{ikr}}{r}$$

  $$\underset{r\to\infty}{=} \left(\sum_l (2l+1)\, P_l(\cos\theta)\, \frac{e^{2i\delta_l} - 1}{2ik} \right) \frac{e^{ikr}}{r}$$

  Therefore, the scattering amplitude is $f_{\mathbf{k}}(\Omega) = \sum_l (2l+1)\, P_l(\cos\theta)\, \dfrac{e^{2i\delta_l} - 1}{2ik}$

Scattering state $|\Psi_{\mathbf{k}}\rangle$: partial–wave expansion

- We have proved: $[\alpha_l = \sqrt{4\pi}\,(2l+1)^{1/2}\, i^l\, e^{i\delta_l}/k]$

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_l \sqrt{4\pi}\,(2l+1)^{1/2}\, i^l e^{i\delta_l}\, \frac{\Psi_{k,l}(r)}{k}\, Y_{l,0}(\hat{\mathbf{r}}) = \sum_l (2l+1)\, P_l(\cos\theta)\, i^l e^{i\delta_l}\, \frac{\Psi_{k,l}(r)}{k}$$

- Finally, restore the role of $\mathbf{k}$ using $\mathbf{k}\cdot\mathbf{r} = kr\cos\theta$, or equivalently $\hat{\mathbf{k}}\cdot\hat{\mathbf{r}} = \cos\theta$

Use the 'addition theorem': $P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}) = \dfrac{4\pi}{2l+1} \displaystyle\sum_{m=-l}^{l} Y^*_{l,m}(\hat{\mathbf{k}})\, Y_{l,m}(\hat{\mathbf{r}})$

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \frac{4\pi}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y^*_{l,m}(\hat{\mathbf{k}})\, Y_{l,m}(\hat{\mathbf{r}})\; i^l\, e^{i\delta_l}\; \Psi_{k,l}(r)$$

where $u_{k,l}(r) = r\,\Psi_{k,l}(r)$ is the (real) solution of:

$$-\frac{\hbar^2}{2m}\, u''_{k,l}(r) + \left(\frac{\hbar^2}{2m}\,\frac{l(l+1)}{r^2} + V(r)\right) u_{k,l}(r) = \frac{\hbar^2 k^2}{2m}\, u_{k,l}(r)$$

which satisfies $u_{k,l}(0) = 0$ and $u_{k,l}(r) \underset{r\to\infty}{=} \sin(kr - l\pi/2 + \delta_l)$

[Messiah, *Quantum Mechanics*, volume II, Wiley (1958), chap. XIX, exercice 4]

Orthogonality of the scattering states $|\Psi_{\mathbf{k}}\rangle$

1. If $|\mathbf{k}_1| \neq |\mathbf{k}_2|$, give a *simple* argument why $\langle \Psi_{\mathbf{k}_1} | \Psi_{\mathbf{k}_2} \rangle = 0$

HINT: The states $|\Psi_{\mathbf{k}_1}\rangle$ and $|\Psi_{\mathbf{k}_2}\rangle$ are both eigenstates of the same Hamiltonian H.

From now on, we assume that $|\mathbf{k}_1|$ and $|\mathbf{k}_2|$ are arbitrarily close (their directions may differ)

2. Show that, for a given l, the radial wavefunctions $u_{k,l}(r)$ satisfy:

$$\int_0^\infty dr\, u_{k_1,l}(r)\, u_{k_2,l}(r) \;=\; \frac{1}{4}\, \delta\left(\frac{k_1 - k_2}{2\pi}\right)$$

HINTS: The radial waves are defined for $r > 0$; exploit their asymptotic behaviour.

3. Use the partial wave expansion to show that: $\langle \Psi_{\mathbf{k}_1} | \Psi_{\mathbf{k}_2} \rangle \;=\; \delta\left(\frac{\mathbf{k}_1 - \mathbf{k}_2}{2\pi}\right)$

HINTS: The spherical harmonics satisfy:

the orthonormality condition $\int \sin\theta\, d\theta\, d\phi\; Y^*_{l_1,m_1}(\hat{\mathbf{r}})\, Y_{l_2,m_2}(\hat{\mathbf{r}}) \;=\; \delta_{l_1,l_2}\, \delta_{m_1,m_2}$

the completeness relation $\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y^*_{l,m}(\hat{\mathbf{k}}_1)\, Y_{l,m}(\hat{\mathbf{k}}_2) \;=\; \delta(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)$

Contact potential

also called:

Zero–range potential

Universal regime for low–energy scattering and bound states

[Huang, *Statistical Mechanics*, Wiley (1963), §10.5]

[Pitaevskii & Stringari, *Bose–Einstein Condensation and Superfluidity*, OUP (2016), §9.2]

Dirac peak 'potential': ambiguous $E{=}0$ scattering state

- Consider the 'potential' $V_\delta(r) = g\,\delta(\mathbf{r})$, which is spherically symmetric

  Look for the zero–energy scattering state: $\Psi_0(r) \underset{r\to\infty}{=} 1 - a/r$

  Reduced mass $m_{\rm red} = m/2$ for two particles with the same mass

- Introduce $u_0(r) = r\,\Psi_0(r)$: $-\dfrac{\hbar^2}{m}\,u_0''(r) + V_\delta(r)\,u_0(r) = 0$ with $u_0(r) \underset{r\to\infty}{=} r - a$

  For $r > 0$, $V_\delta(r)$, plays no role, so that $u_0''(r) = 0$ and $u_0(r) = r - a$

  $$\Psi_0(r) = 1 - a/r$$

- Schrödinger equation: $$-\frac{\hbar^2}{m}\nabla^2\Psi_0(r) \quad + \quad g\,\delta(\mathbf{r})\,\Psi_0(r) \quad = \quad 0$$

  Inject $\Psi_0(r)$ and use $\nabla^2(1/r) = -4\pi\,\delta(\mathbf{r})$ (Poisson formula in electrostatics)

  $$\delta(\mathbf{r})\left(-\frac{4\pi\hbar^2\,a}{m} + g(1 - a/r)\right) = 0$$ **cannot be satisfied for all $r \geq 0$**

Contact potential: formulation as a pseudo–potential

- The difficulty comes from the non–regular part $-a/r$: remove it using a derivative

$$\langle \mathbf{r} | V_{\text{pseudo}} | \Psi \rangle \quad = \quad g\,\delta(\mathbf{r})\,\frac{\partial [r\,\Psi(\mathbf{r})]}{\partial r}$$

- Expand the wavefunction $\Psi(\mathbf{r}) = \sum_{l,m} \Psi_{l,m}(r)\; Y_{l,m}(\theta,\phi)$ onto spherical harmonics

Important: Domain of the Hamiltonian:

Wavefunctions $\Psi(\mathbf{r})$ such that all $r\,\Psi_{l,m}(r)$ are **finite** for $r \to 0$

Different from the case of a regular potential, for which $r\,\Psi_{l,m}(r) \underset{r\to 0}{=} 0$

- V_{pseudo} coincides with V_δ for all wavefunctions $\Psi_{l,m}(r)$ that are regular at $r = 0$

$$g\,\delta(\mathbf{r})\frac{\partial}{\partial r}\left[r\Psi_{l,m}(r)\right] \;=\; g\,\delta(\mathbf{r})\left[\Psi_{l,m}(r) + r\Psi'_{l,m}(r)\right] \;=\; g\,\delta(\mathbf{r})\,\Psi_{l,m}(0)$$

- Wavefunctions **diverging** like $1/r$: $\Psi_{l,m}(r) = \chi_{l,m}(r)/r$ with χ regular at $r = 0$

$$g\,\delta(\mathbf{r})\frac{\partial}{\partial r}\left[r\Psi_{l,m}(r)\right] \;=\; g\,\delta(\mathbf{r})\,\chi'_{l,m}(r) \;=\; g\,\delta(\mathbf{r})\,\chi'_{l,m}(0)$$

$\langle r | V_{\text{pseudo}} | \Psi_{l,m} \rangle \;=\; g\,\delta(\mathbf{r})\,\chi'_{l,m}(0)$ is also well defined.

Pseudo–potential: scattering length

$$\langle \mathbf{r} | V_{\text{pseudo}} | \Psi \rangle = g\,\delta(\mathbf{r})\,\frac{\partial [r\,\Psi(\mathbf{r})]}{\partial r}$$

- The pseudopotential V_{pseudo} is spherically symmetric

  Look for the zero–energy scattering state: $\Psi_0(r) \underset{r\to\infty}{=} 1 - a/r$

  Reduced mass $m_{\text{red}} = m/2$ for two particles with the same mass

- Introduce $u_0(r) = r\,\Psi_0(r)$: $-\frac{\hbar^2}{m}\,u_0''(r) + V_{\text{pseudo}}(r)\,u_0(r) = 0$ with $u_0(r) \underset{r\to\infty}{=} r - a$

  For $r > 0$, $V_{\text{pseudo}}(r) = 0$, so that $u_0''(r) = 0$ and $u_0(r) = r - a$

  $\Psi_0(r) = 1 - a/r$

- Schrödinger equation: $-\frac{\hbar^2}{m}\,\nabla^2\Psi_0(r) + g\,\delta(\mathbf{r})\,\frac{\partial}{\partial r}[r\,\Psi_0(r)] = 0$

  Inject $\Psi_0(r)$ and use $\nabla^2(1/r) = -4\pi\,\delta(\mathbf{r})$ (Poisson formula in electrostatics)

  $\delta(\mathbf{r})\left(-\frac{4\pi\hbar^2\,a}{m} + g\right) = 0,$ so that $g = \frac{4\pi\hbar^2\,a}{m}$ as expected.

Pseudo–potential: bound state (1/2)

- Spherical symmetry: look for a bound state ψ_l which is an eigenstate of $\mathbf{l}^2$ and l_z

  Bound state means negative energy: $E = -\hbar^2\kappa^2/m$ with $\kappa > 0$

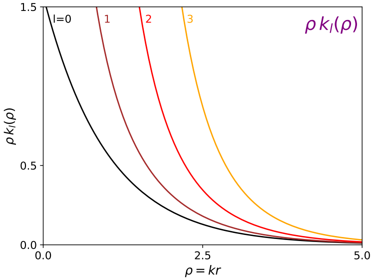
  Schrödinger equation for $r > 0$: V_{pseudo} plays no role

$$-\frac{\hbar^2}{m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\psi_l) + \frac{\hbar^2}{m}\frac{l(l+1)}{r^2}\psi_l = -\frac{\hbar^2\kappa^2}{m}\psi_l$$

- Change variable to $\rho = \kappa r$: $$-\frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}(\rho\,\psi_l) + \frac{l(l+1)}{\rho^2}\psi_l = -\psi_l$$

- Normalisable solutions are proportional to the spherical Bessel function $k_l(\rho)$: $\psi_l(r) = \alpha\, k_l(\kappa\, r)$

$$k_l(\rho) \underset{\rho\to 0}{=} \frac{\pi}{2}\frac{(2l-1)!!}{\rho^{l+1}} \quad \text{and} \quad k_l(\rho) \underset{\rho\to\infty}{=} \frac{\pi}{2}\frac{e^{-\rho}}{\rho}$$



- Domain of V_{pseudo}: $r\psi_l$ must be finite for $r \to 0$

Hence, there are only s–wave bound states (if any): $l = 0$ and $\psi_0(r) = \beta\,\frac{e^{-\kappa r}}{r}$

Pseudo–potential: bound state (2/2)

$\psi_0(r) = \beta \exp(-\kappa r)/r$ with $E = -\hbar^2\kappa^2/m$ and $\kappa > 0$

- *s*–wave Schrödinger equation: $-\dfrac{\hbar^2}{m}\nabla^2\psi_0 + \dfrac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})\dfrac{\partial}{\partial r}[r\,\psi_0(r)] = -\dfrac{\hbar^2\kappa^2}{m}\psi_0$

- Behaviours for $r \to 0$: [If $f(r)$ is regular at $r = 0$, $\nabla^2 f(r) = (1/r)\partial^2(rf)/\partial r^2$

  $\psi_0(r) = \beta(1/r - \kappa) + O(r)$, $\nabla^2\psi_0 = -4\pi\beta\,\delta(\mathbf{r}) + O(1/r)$, $\partial(r\,\psi_0)/\partial r = -\beta\kappa + O(r)$

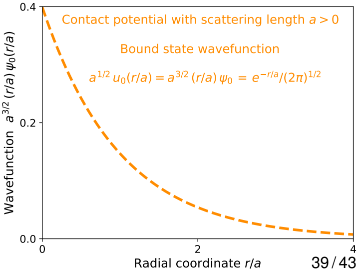
  Inject them in the Schrödinger equation: $(1 - \kappa a)\,\delta(\mathbf{r}) = O(1/r)$, so that $\kappa = 1/a$

- $\kappa > 0$, therefore: no bound state if $a < 0$, a single bound state if $a > 0$

  The bound state represents a molecule: it only exists for repulsive interactions.

$$\psi_0(r) = \frac{1}{(2\pi a^3)^{1/2}}\,\frac{\exp(-r/a)}{r/a}$$

- $r\,\psi_0(r)$ is finite but non–zero for $r \to 0$
- spatial extent set by scattering length a
- energy $E = -\hbar^2/(ma^2)$



Pseudo–potential: scattering state with energy $E > 0$

- The incident wavevector is $\mathbf{k}$ such that $E = \hbar^2 k^2/m$ [reduced mass $m_{\text{red}} = m/2$]

  Expand the scattering state $\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_l \Psi_l(r)\, Y_{l,0}(\theta,\phi)$ into partial waves

V_{pseudo} plays no role for $r > 0$: $\Psi_l(r)$ satisfies the same equation as the plane wave $\Phi_{\mathbf{k}}$

Solution: linear combination of spherical Bessel functions $\Psi_l(r) = \alpha_l\, j_l(kr) + \beta_l\, y_l(kr)$

- Behaviour for small r: $j_l(\rho) \underset{\rho\to 0}{=} \dfrac{\rho^l}{(2l+1)!!}$ and $y_l(\rho) \underset{\rho\to 0}{=} -\dfrac{(2l-1)!!}{\rho^{l+1}}$

  Domain of V_{pseudo}: $r\,\Psi_l(r)$ must be finite for $r \to 0$, therefore $\beta_l = 0$ for all $l \geq 1$

Only the s–wave component is scattered! [Plane wave: $r\,\Phi_l \underset{r\to 0}{=} 0$, so that even $\beta_0 = 0$]

- Scattering state for all $r > 0$: $\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \dfrac{a}{1+ika}\dfrac{e^{ikr}}{r}$

  HINTS: First, show that the s–wave component $u_0(r) = \sin(kr+\delta_0)$ with $\tan\delta_0 = -ka$

  Then, use $f = f_0 = \dfrac{e^{2i\delta_0}-1}{2ik}$ along with the identity $e^{2i\delta_0} = \frac{1+i\,\tan\delta_0}{1-i\,\tan\delta_0}$

Universality for low–energy scattering & bound states

For distances greater than the potential range *b*,

The scattering length a fully dictates the behaviour of ...

- **Low–energy** scattering states

zero–energy scattering state: $\Psi_0(r) \underset{r \gg b}{=} 1 - a/r$

low –energy scattering state: $\Psi_{l=0}(r) \underset{r \gg b}{=} \dfrac{\sin[k(r-a)]}{kr}$ (see qu. 13–14)

- **Weakly** bound states

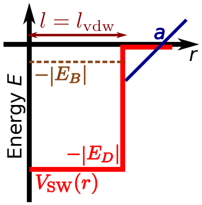
wavefunction $\psi_0(r) = \dfrac{1}{(2\pi\, a^3)^{1/2}} \dfrac{\exp(-r/a)}{r/a}$, spatial extent $a \gg b$ (halo), energy $\varepsilon = -\dfrac{\hbar^2}{m\, a^2}$

Beware: No universality for deeper bound states

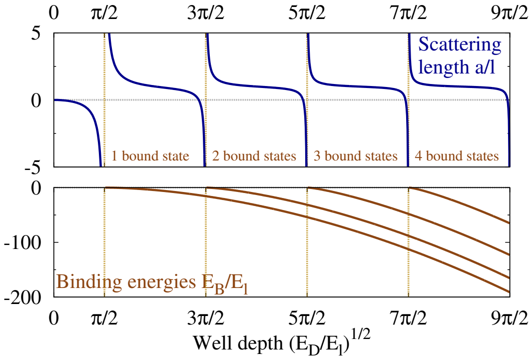
- In the universal regime, for $r \gg b$,

all wavefunctions coincide with the ones calculated using the contact potential.

Universality on an example: the square well potential

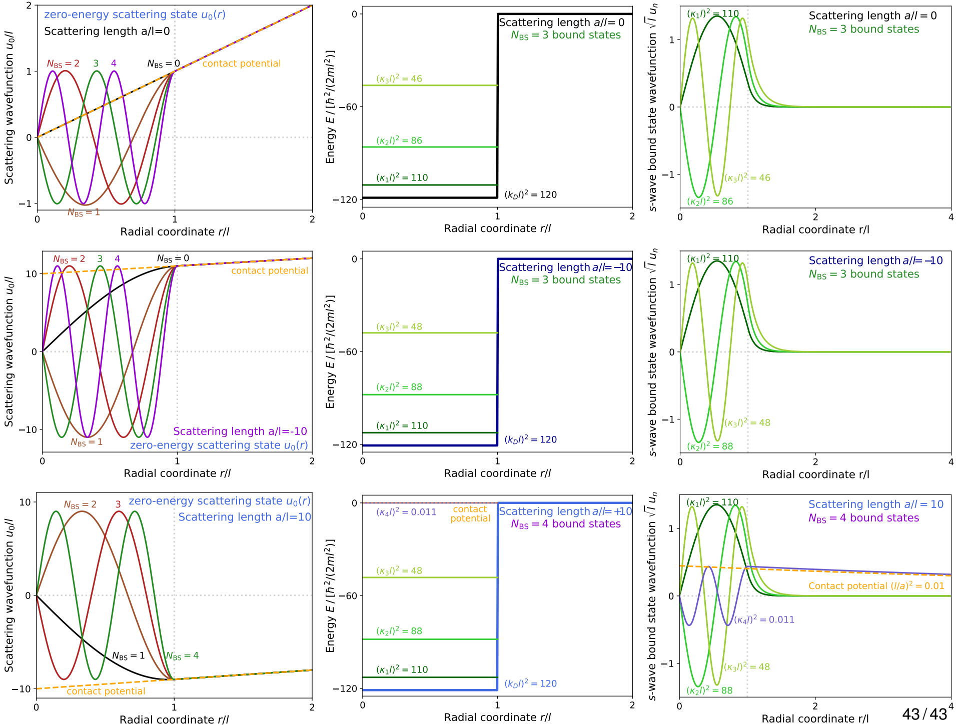


Unit of energy: $E_l = \hbar^2/(2ml^2)$



- Next slide: scattering and bound–state wavefunctions for various values of a/l obtained in the cases where the well supports 3 bound states or 4 bound states and compares them to the predictions of the contact potential.

The considered wavefunctions are all s–wave; plotted quantities: $u_0(r) = r\Psi_0(r)$ or $u_n(r) = r\psi_n(r)$


zero-energy scattering state $u_0(r)$
Scattering length a/l=0
$N_{BS}=2$
3
4
$N_{BS}=0$
contact potential
$N_{BS}=1$
Scattering wavefunction u_0/l
Radial coordinate r/l
Scattering length $a/l=0$
$N_{BS}=3$ bound states
$(\kappa_3 l)^2=46$
$(\kappa_2 l)^2=86$
$(\kappa_1 l)^2=110$
$(k_D l)^2=120$
Energy E / $[\hbar^2/(2ml^2)]$
$(\kappa_1 l)^2=110$
$(\kappa_3 l)^2=46$
$(\kappa_2)^2=86$
s-wave bound state wavefunction $\sqrt{l}\,u_n$
Radial coordinate r/l
Scattering length a/l=-10
zero-energy scattering state $u_0(r)$
Scattering length $a/l=-10$
$N_{BS}=3$ bound states
$(\kappa_3 l)^2=48$
$(\kappa_2 l)^2=88$
$(\kappa_1 l)^2=110$
$(k_D l)^2=120$
$(\kappa_3 l)^2=48$
$(\kappa_2)^2=88$
Scattering length a/l=10
$N_{BS}=4$
Scattering length $a/l=+10$
$N_{BS}=4$ bound states
$(\kappa_4 l)^2=0.011$
contact potential
Scattering length $a/l=10$
Contact potential $(l/a)^2=0.01$
$(\kappa_4 l)^2=0.011$