ADVANCED QUANTUM MECHANICS

TUTORIALS 2024–2025

David Papoular

Laboratoire de Physique Théorique et Modélisation, Univ. Cergy–Pontoise

david.papoular@u-cergy.fr

Please ask me MANY questions!

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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: DIGEST

- 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*, 5th 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 $k=\omega/c$

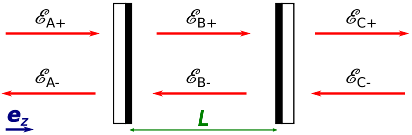
  All solutions $\mathbf{E}(z,t)$ propagating along z are linear combinations of plane waves:

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

- 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: $\mathbf{E} = \mathbf{e}\,\mathcal{E}(\mathbf{r},t)$

- 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:

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

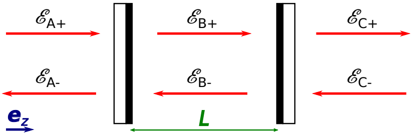
- Propagation equation is 2nd–order: $\dfrac{d^2\mathbf{E}}{dz^2} = \dfrac{\omega^2}{c^2}\mathbf{E}$ so 2 conditions are required

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

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

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

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



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

- 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 $\exp(\pm ikL)$

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

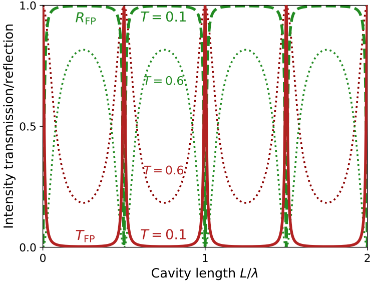
- Transmission and reflection coefficients for the Fabry–Pérot (FP) cavity:

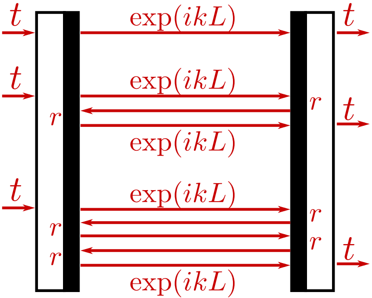
$$t_{\mathrm{FP}} = \frac{\mathscr{E}_{C+} \exp(ikL)}{\mathscr{E}_{A+}} = \frac{t^2 \exp(ikL)}{1 - r^2 \exp(2ikL)} \quad \text{and} \quad r_{\mathrm{FP}} = \frac{\mathscr{E}_{A-}}{\mathscr{E}_{A+}} = r\,\frac{1 - \exp(2ikL)}{1 - r^2 \exp(2ikL)}$$

Fabry–Pérot: resonant cavity (qu. 4)

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

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





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

- 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

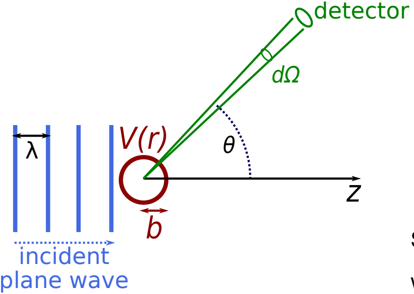
For $r \to \infty$, the interaction potential $V(\mathbf{r})$ is negligible compared to the kinetic energy

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.

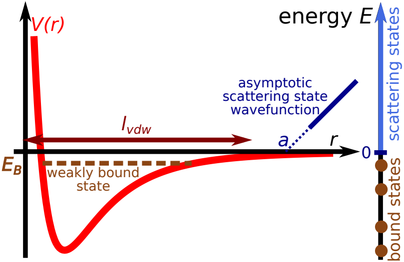
- Unlike for bound states, the energy is known before calculating $|\Psi\rangle$: $E = \hbar^2k^2/(2m)$
- **This is not an initial value problem!**

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 $r \to \infty$

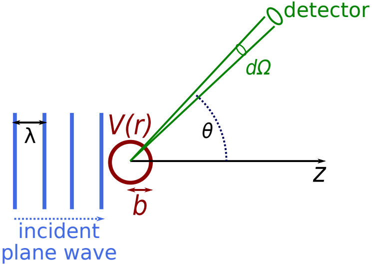
  Labelled by a discrete index n, $\int d^3r\, |\psi_n|^2 = 1$,

- 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 $v\,dS$

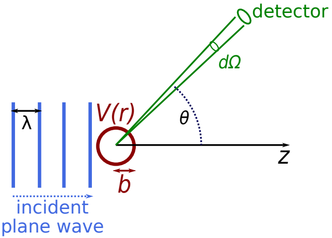
- The scattering state $|\Psi_{\mathbf{k}}\rangle$ and amplitude $f_{\mathbf{k}}(\Omega)$ are fully determined by this choice

  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: $\Psi_{\mathbf{0}}(r) \underset{r\to\infty}{=} 1 - \frac{a}{r}$

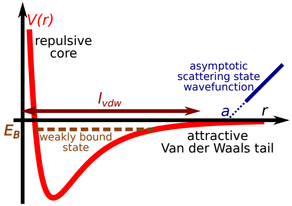
- **In a dilute system,** (i.e. holds in a gas)

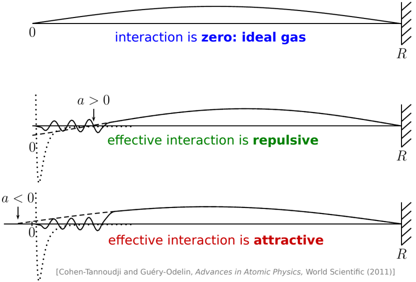
  the **scattering length** a encodes all properties of low–energy scattering

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

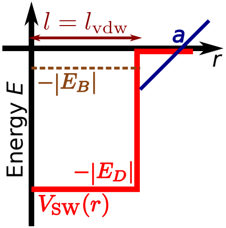




[Cohen-Tannoudji and Guéry-Odelin, *Advances in Atomic Physics*, World Scientific (2011)]

- 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



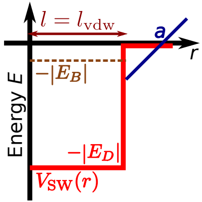
- Replace the potential

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: $\nabla^2\Psi_0(r) = \dfrac{1}{r}\dfrac{d^2}{dr^2}(r\,\Psi_0)$

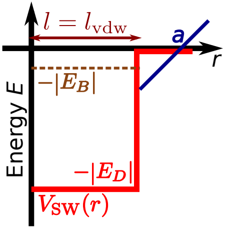
  Zero–energy Schrödinger equation: $0 = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dr^2}(r\Psi_0) + V_{\mathrm{SW}}(r)\,(r\Psi_0)$

  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 $V_{\rm SW}(r)$:

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

- 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)

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

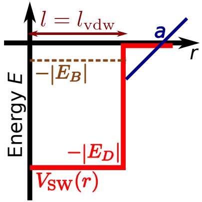
- $H = \dfrac{\mathbf{p}^2}{2m} + V(r)$ commutes with $\mathbf{l}$: look for eigenstates $|\Psi_{n,l,m}\rangle$ shared by H, $\mathbf{l}^2$, l_z

  $l^2\,|\Psi_{n,l,m}\rangle = \hbar^2 l(l+1)\,|\Psi_{n,l,m}\rangle$ 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 $u_n(0) = 0$

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



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

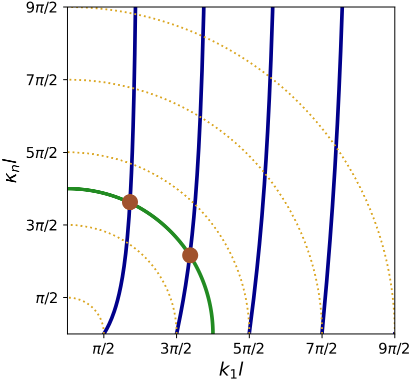
  $u_n''(r) + k_1^2 u_n(r) = 0$ with $k_1^2 = k_D^2 - \kappa_n^2 \ge 0$

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



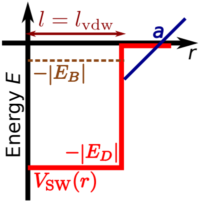
- Graphical solution: look for the intersections of the blue and green curves in the $(k_1 l, \kappa_n l)$ quarter–plane $(k_1 > 0,\ \kappa_n > 0)$
- If $(n - 1/2)\,\pi < k_D\, l < (n + 1/2)\,\pi$, n intersections, hence, n bound states

  $n = 2$ on the figure

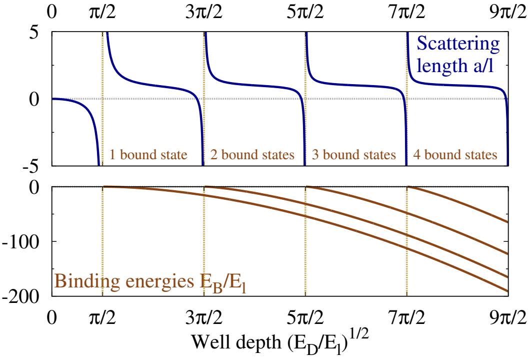
- For every $k_D l = (n + 1/2)\,\pi$, a new bound state appears

  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

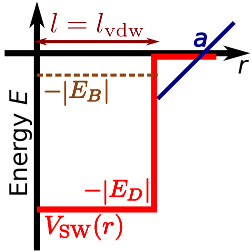
  The analogy has limitations: the spatial extent of the bound state is $a \gg l$
- This is a general property known as LEVINSON'S theorem:

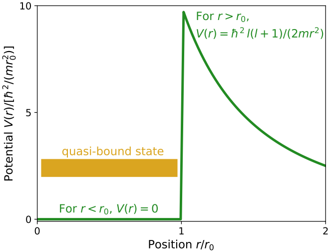
  For any spherically–symmetric potential $V(r)$ (smooth and well–behaved for $r \to 0$ and $r \to +\infty$), the scattering length a diverges each time a new bound state appears

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

Fabry–Pérot analogue: scattering resonance

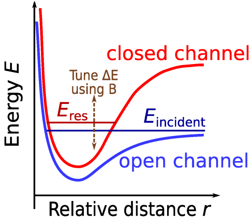
- Simplest example: one scattering channel **‘shape resonance’**

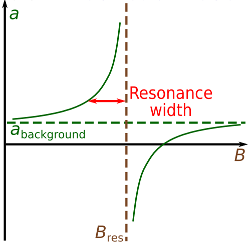




[Messiah, *Quantum Mechanics*, Wiley (1958), vol. I, chapter 10, §15]

- 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

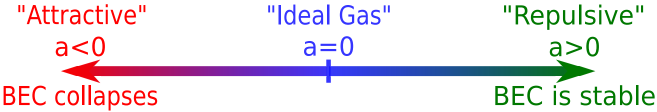
[Castin & Werner, in *The BCS–BEC crossover and the unitary Fermi gas*,
Lecture Notes in Physics **836**, Zwerger (ed), Springer (2012)]

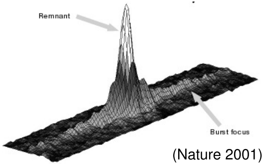
Tuning the interaction between many bosonic atoms

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

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

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

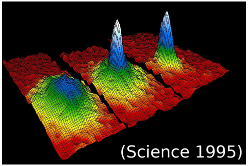




(Nature 2001)

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

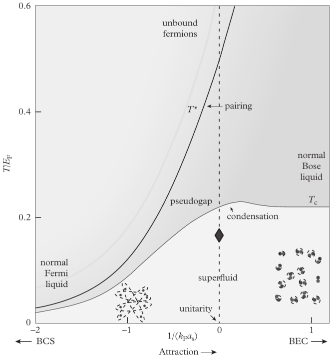
- In order to beat Pauli's exclusion, we need at least
  2 different species (e.g. $^{6}\mathrm{Li}$, $^{40}\mathrm{K}$) or 2 internal states of the same atom ($|\uparrow\rangle$, $|\downarrow\rangle$)

- 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)]

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 $m_{\mathrm{red}} = m/2$ 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: $-\dfrac{\hbar^2}{m}\,\nabla^2\Psi_0(r) + g\,\delta(\mathbf{r})\,\Psi_0(r) = 0$

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

  $$\delta(\mathbf{r})\left(-\frac{4\pi\hbar^2 a}{m} + g(1 - a/r)\right) = 0$$ **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

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

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

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

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

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

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

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

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

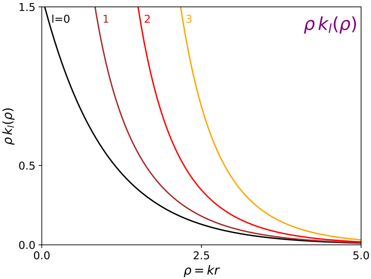
$$-\frac{\hbar^2}{m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\psi_l) \quad + \quad \frac{\hbar^2}{m}\frac{l(l+1)}{r^2}\psi_l \quad = \quad -\frac{\hbar^2\kappa^2}{m}\psi_l$$

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

- 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 $\psi_0(r) = \beta\,\frac{e^{-\kappa r}}{r}$

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

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 $r = 0$, $\nabla^2 f(r) = (1/r)\partial^2(rf)/\partial r^2$

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

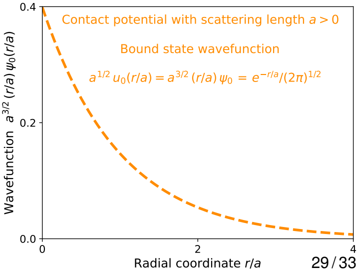
  Inject them in the Schrödinger equation: $(1 - \kappa a)\,\delta(\mathbf{r}) = O(1/r)$, so that $\kappa = 1/a$

- $\kappa > 0$, 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 $E = -\hbar^2/(ma^2)$



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

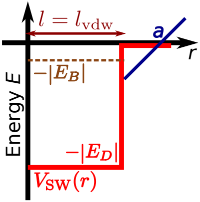
wavefunction $\psi_0(r) = \dfrac{1}{(2\pi\, a^3)^{1/2}} \dfrac{\exp(-r/a)}{r/a}$, spatial extent $a \gg b$ (halo), energy $\varepsilon = -\dfrac{\hbar^2}{m\, a^2}$

Beware: No universality for deeper bound states

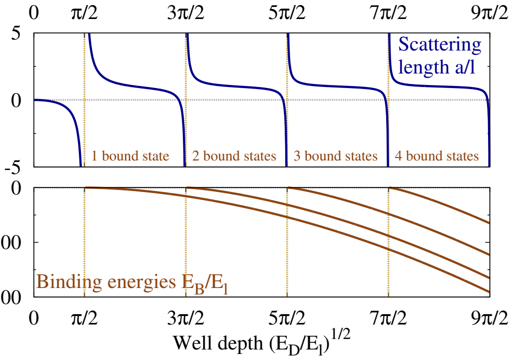
- In the low–energy universal regime, for $r \gg b$,

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

Universality on an example: the square well potential

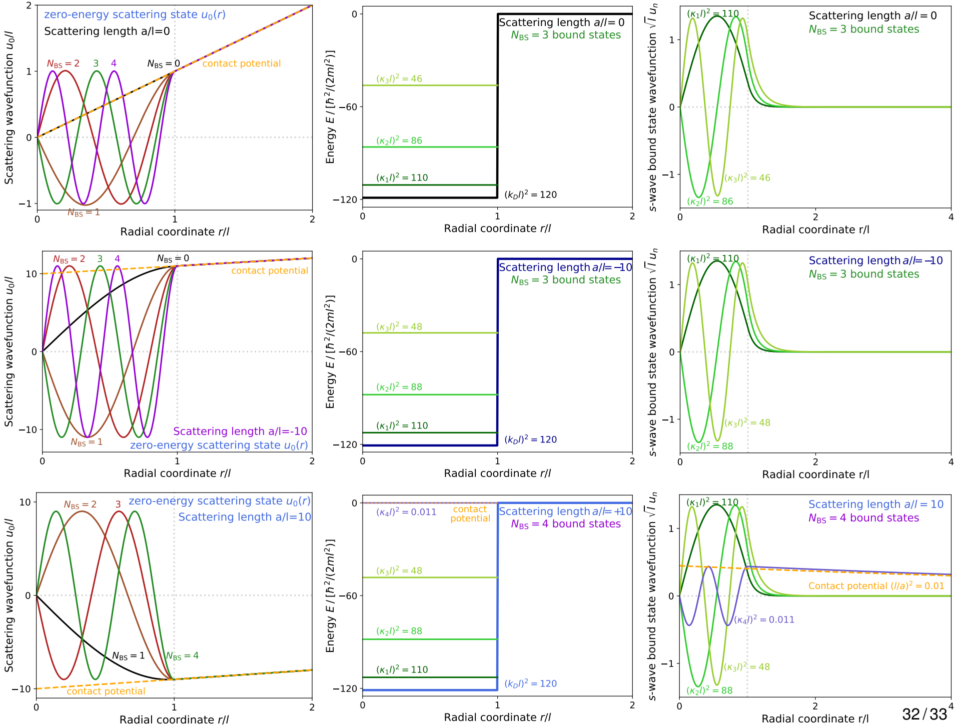


Unit of energy: $E_l = \hbar^2/(2ml^2)$



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

Thanks for your regular attendance!

Happy Holidays!

Good luck, lots of success and enjoyment!