Cold Atoms in Optical Lattices 2

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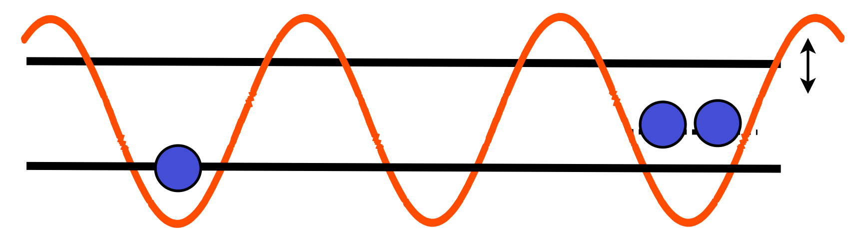
Outline of Lectures

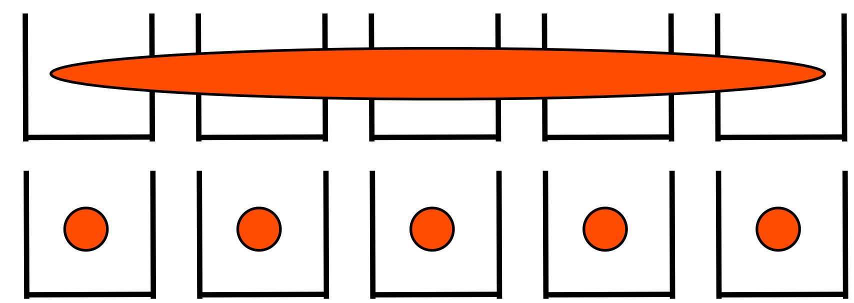
Now:

- Optical Lattices
- Band Structure, Bloch & Wannier functions
- Bose-Hubbard model



Later:

- Phase diagram of the Bose-Hubbard model: Superfluid, Mott-Insulator
- Single-Particle density matrix & correlations

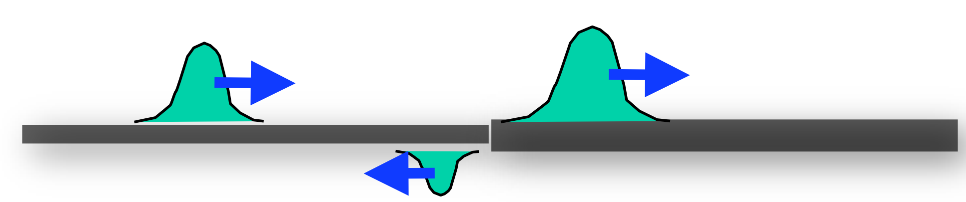


Wednesday:

- Microscopic model for interactions
- Zero-range pseudopotential and its properties

Friday:

- Transport of atoms in optical lattices in 1D (Andreev Reflections, superfluidity)
- Dynamics of three-body loss in an optical lattice

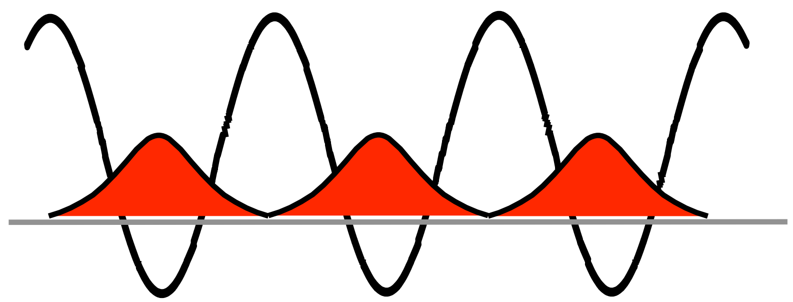


Problem Classes:

- Today: Quasimomentum in the Bose-Hubbard model
- Tomorrow: Two particles on a lattice

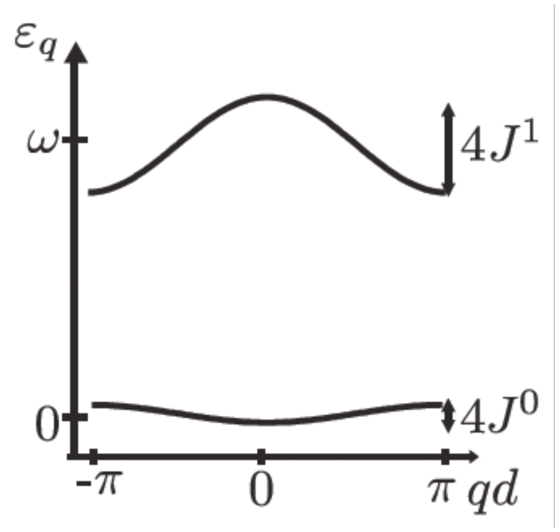
Bose-Hubbard Model: Summary

$$\hat{H} = \int d\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\hat{\Psi}(\mathbf{x}) + \frac{g}{2}\int d\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$



Wannier functions

$$\psi(\vec{x}) = \sum_\alpha w(\vec{x} - \vec{x}_\alpha)\, b_\alpha$$



Assume:
- Only lowest band
- Only nearest neighbour tunneling
- Only onsite interactions

$$J = -\int dx\, w_0(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\sin^2(k_l x)\right) w_0(x-a),$$

$$U = g\int d\mathbf{x}\, |w_0(\mathbf{x})|^4,$$

$$\epsilon_i = \int d\mathbf{x}\, |w_0(\mathbf{x}-\mathbf{x}_i)|^2\, (V(\mathbf{x}-\mathbf{x}_i)),$$

$$\longrightarrow \quad H = -J\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j + \sum_i \epsilon_i\hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \qquad k_B T, J, U \ll \hbar\omega$$

D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys Rev. Lett. **81**, 3108 (1998)

Microscopic Model for Cold Bosons

- In terms of second quantised field operators $\hat{\psi}(\mathbf{r})$, the many-body Hamiltonian for a Bose gas, including the effects of an external trapping potential and two-body interactions may be written as

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d^3r \int d^3r'\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r}')\, V(\mathbf{r}'-\mathbf{r})\, \hat{\psi}(\mathbf{r}')\, \hat{\psi}(\mathbf{r})$$

- Here, $V_{ext}(\mathbf{r})$ is an external potential (e.g., a magnetic trapping potential, or potential due to an AC-Stark shift from interaction with laser light).
- $V(\mathbf{r}' - \mathbf{r})$ is the two-body interaction Hamiltonian. Treating only two-body interactions is valid provided that the gas is sufficiently dilute that higher order interactions are not relevant on the timescale of the experiment.
- For low energy collisions between distinguishable particles or Bosons, we can write

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{g}{2}\int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}(\mathbf{r})\, \hat{\psi}(\mathbf{r})$$

- Note: The second-quantised field operators obey the commutation relation

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{g}{2}\int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}(\mathbf{r})\, \hat{\psi}(\mathbf{r})$$

- That these operators represent Bosons is an approximation: our atoms are actually composed of Fermions. In fact, the commutator is actually

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}') - D(\mathbf{r}-\mathbf{r}')$$

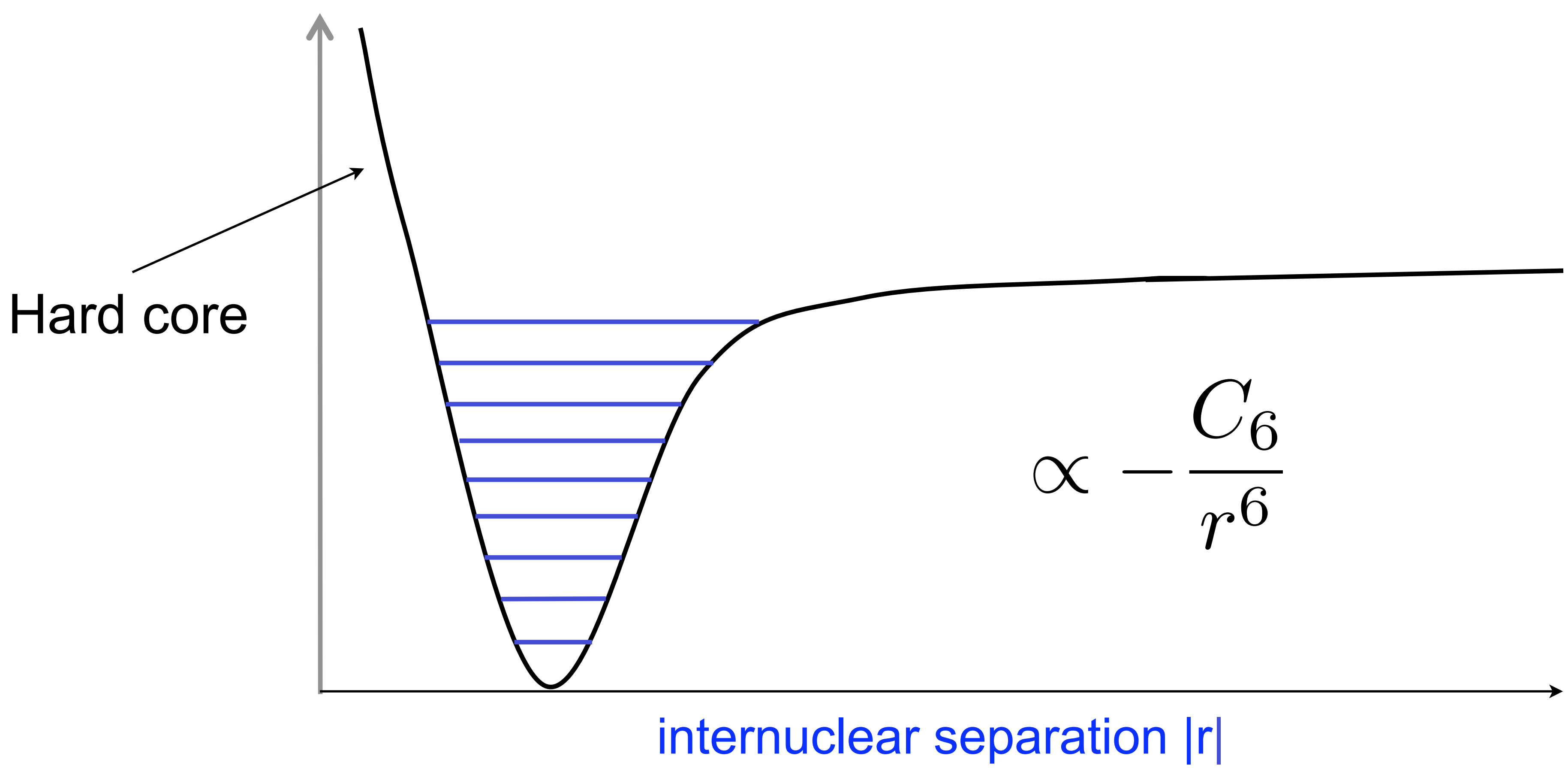
  where the correction $D(\mathbf{r}-\mathbf{r}')$ is small provided that $|\mathbf{r}-\mathbf{r}'| \gg b_0$, where b_0 is the typical extent of the electronic wavefunctions for a single atom.

- Thus, these corrections play a small role provided that the typical size of the atoms (The Bohr radius, $\sim$0.05 nm) is small compared with the typical separation between atoms in the condensate (typically $>$10nm, even in an optical lattice).

- EXERCISE: Try computing $D(\mathbf{r}-\mathbf{r}')$ for the Hydrogen atom, $\hat{\psi}_H(\mathbf{R}) \approx \int d^3r\ \phi(\mathbf{r})\, \hat{\psi}_e(\mathbf{R}+\mathbf{r})\hat{\psi}_p(\mathbf{R})$ (where we take $m_e/m_p \approx 0$)

Interactions in a dilute Bose Gas

- In thermal equilibrium typical BECs in atomic gases would be solid (crystalline)
- Density of gas is sufficiently small that 3-body collisions are rare, and gas is metastable with lifetimes of the order of seconds
- Also because 3-body collisions are rare, interactions may be treated as two-body scattering.
- We see this metastability from the Born-Oppenheimer curve for the interaction potential, where the unbound state is a metastable state.



Range:

$$b \sim \left(\frac{m C_6}{\hbar^2} \right)^{1/4}$$

Why use a pseudopotential?

- In the limit of low energies, the scattering properties are universal, and depend essentially on 1 parameter, the scattering length a. The details of the scattering potential are, in this sense not important. The scattering length will be measured experimentally, and this is the only data really required to describe 2-body interactions in the system.
- At the same time, it is difficult to determine the real potential $V(r)$ precisely, and difficult to perform calculations with it.
- Any small error in $V(r)$ could significantly change the scattering properties, when really the most relevant information is simply the value for the scattering length produced by the potential.
- The weakly interacting Bose gases we deal with are metastable. We thus cannot perform calculations assuming thermal equilibrium using the real potential.
- Because $V(r)$ is strongly repulsive at short distances and has many bound states, the Born approximation (1st order perturbation theory) is not valid when used with the real potential.
- We thus replace exact interaction potential with a potential having the same scattering properties at low energy (i.e., the same scattering length), but that is treatable in the Born approximation and easier in general to work with mathematically.

- The pseudopotential with only the one necessary parameter is the zero-range pseudopotential, originally used by Fermi.

$$\langle \mathbf{r}|\, V(\mathbf{r})\, |\psi(\mathbf{r})\rangle = g\,\delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$$

with

$$g = \frac{2\pi\hbar^2 a}{m_r} = \frac{4\pi\hbar^2 a}{m}$$

References:

- E. Fermi, La Ricerca Scientifica, VII-II (1936), 1352.
- K. Huang and C. N. Yang, Phys. Rev. 105 (1957), 767.

- K. Huang, Statistical Mechanics, Wiley, New York, 1963.
- “Bose-Einstein Condensation in Atomic Gases: simple theoretical results” Yvan Castin, http://www.arxiv.org/abs/cond-mat/0105058

- R. Stock, A. Siberfarb, E. L. Bolda and I. H. Deutsch, PRL 94 (2005), 023202.
- A. Derevianko, PRA 72 (2005), 044701.
- Z. Idziaszek and T. Calarco: PRL 96 (2006), 013201.
- L. Pricoupenko, PRA 73 (2006), 012701.
- F. Stampfer and P. Wagner, J. Mathematical Analysis and Applications 342 (2008), 202

Results from Scattering Theory

- We can show that at large distances from the scattering centre, $r = |\mathbf{r}| \gg b$, where b is the range of the potential, the outgoing scattering wavefunctions for a local potential $V(\mathbf{r})$ are written as the sum of an incoming plane wave and an outgoing spherical wave,

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}.\mathbf{r}} + f(\mathbf{k},\mathbf{k}')\frac{\mathrm{e}^{ikr}}{r}$$

$$f(\mathbf{k},\mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i\mathbf{k}'.\mathbf{r}'}\ V(\mathbf{r}')\,\psi_{\mathbf{k}}^{(+)}(\mathbf{r}')$$

with $m_r = m_1 m_2/(m_1 + m_2)$ the reduced mass,

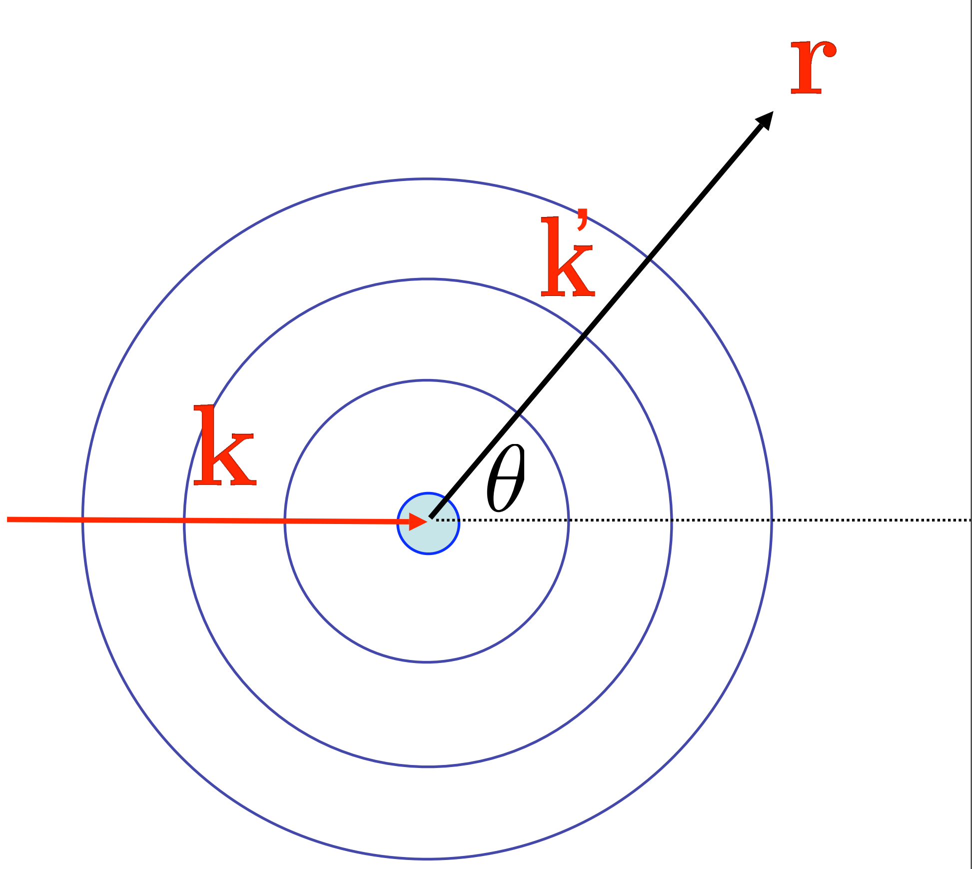
$$r = |\mathbf{r}|, \quad k = |\mathbf{k}| = \sqrt{\frac{2mE}{\hbar^2}}$$

and $\mathbf{k}' = k\frac{\mathbf{r}}{|\mathbf{r}|}$.

- For a spherically symmetric potential, $V(\mathbf{r}) = V(r)$ and

$$f(\mathbf{k},\mathbf{k}') = f(k,\theta)$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) \quad = \quad \mathrm{e}^{i\mathbf{k}.\mathbf{r}} + f(k,\theta)\frac{\mathrm{e}^{ikr}}{r}$$



$$\psi^{(+)}_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathbf{ik.r}} + f(\mathbf{k},\mathbf{k}')\frac{\mathrm{e}^{ikr}}{r}$$

$$f(\mathbf{k},\mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i\mathbf{k}'.\mathbf{r}'}\ V(\mathbf{r}')\,\psi^{(+)}_{\mathbf{k}}(\mathbf{r}')$$

Born Approximation

- It is clear that one can iterate this solution in the sense of a perturbation expansion in the strength of the potential $V(\mathbf{r})$. The first order expansion, in which we substitute the incoming plane wave $\psi^{(+)}_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathbf{ik.r}}$ into the expression for the scattering amplitude yields:

$$\begin{aligned}
f(\mathbf{k},\mathbf{k}') &= -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i\mathbf{k}'.\mathbf{r}'}\ V(\mathbf{r}')\,\psi^{(+)}_{\mathbf{k}}(\mathbf{r}')\\
&\approx -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i(\mathbf{k}'-\mathbf{k}).\mathbf{r}'}\ V(\mathbf{r}') + \frac{m_r^2}{4\pi^2\hbar^4}\int d\mathbf{r}'\int d\mathbf{r}''\mathrm{e}^{-i\mathbf{k}'.(\mathbf{r}'+\mathbf{r}'')}\,V(\mathbf{r}'')\,V(\mathbf{r}')\,\psi^{(+)}_{\mathbf{k}}(\mathbf{r}'')\\
&\approx -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i(\mathbf{k}'-\mathbf{k}).\mathbf{r}'}\ V(\mathbf{r}')
\end{aligned}$$

- This first order expansion is known as the Born approximation.

Partial Wave expansion

- If the potential $V(\mathbf{r}) = V(r)$ is spherically symmetric, then the Hamiltonian commutes with the total angular momentum operator, $\hat{L}$ and $\hat{L}^2$.
- We can expand the wavefunction as a sum of states of definite angular momentum as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \frac{\chi_{kl}(r)}{r}$$

where we have chosen the incoming axis to be the z-direction, $P_l(x)$ is a Legendre Polynomial and the scattering amplitude can be expressed as

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

and the radial functions are solutions of the radial Schrödinger equation

$$\frac{d^2\chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2m_r}{\hbar^2}[E - V(r)]\chi_{kl} = 0$$

with $E = \hbar^2 k^2/(2m_r)$.

- For $V(r) = 0$, the general solution to the radial Schrödinger equation,

$$\frac{d^2\chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2m_r}{\hbar^2}[E - V(r)]\chi_{kl} = 0$$

  is given in terms of the so-called spherical Bessel and Von Neumann functions as

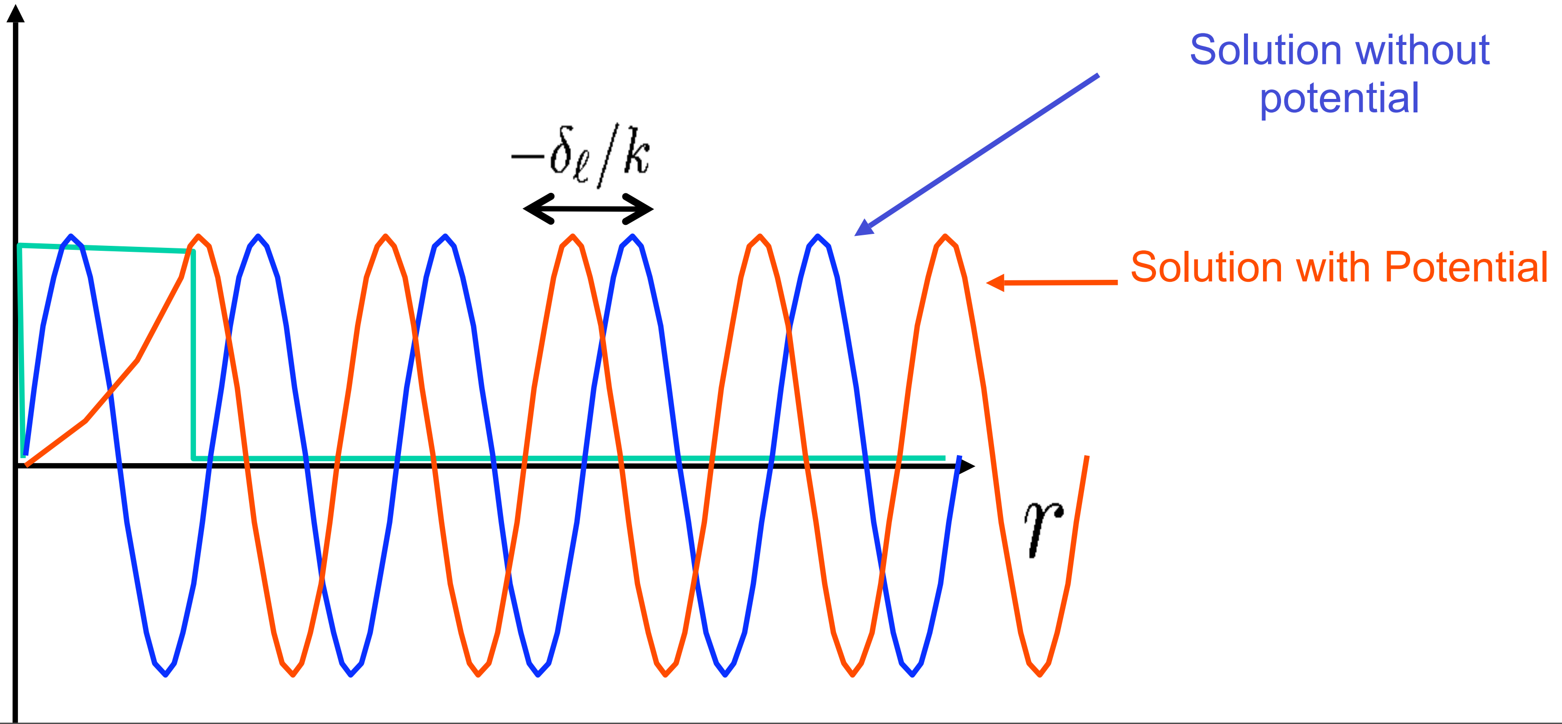
$$\chi_{kl} = A_l[\hat{j}_l(kr)\cos\delta_l + \hat{n}_l(kr)\sin\delta_l]$$

  which reduces at large distances to

$$\chi_{kl}(r) = A_l[\sin(kr - \pi l/2)\cos\delta_l + \cos(kr - \pi l/2)\sin\delta_l] = A_l \sin\left(kr - \frac{\pi l}{2} + \delta_l\right)$$

  where $\delta_l(k)$ are the scattering phase shifts.

- These scattering phase shifts describe the full details of the scattering process, and are in general dependent on both the scattering potential and incident energy.



Scattering from a Hard Sphere

- We consider the simple example of scattering from a hard sphere,

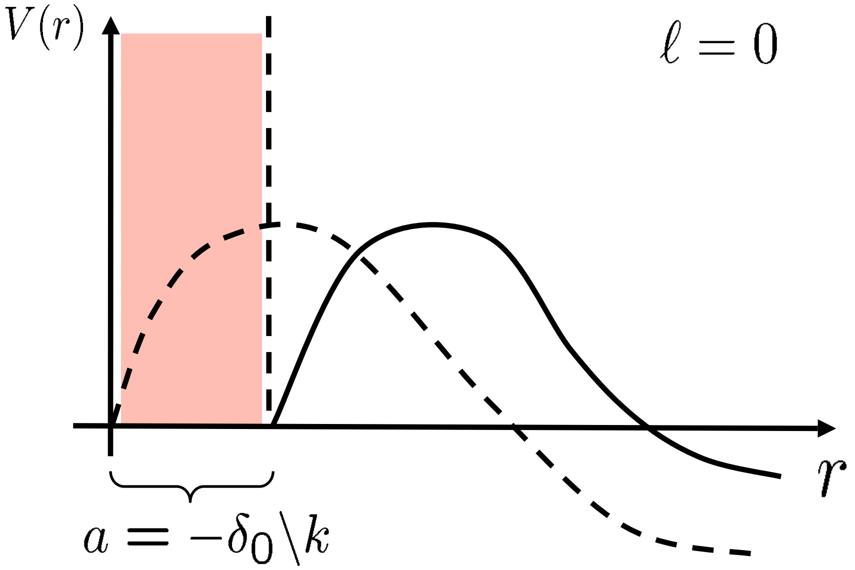
$$V(r) = \begin{cases} \infty, & r \leq a \\ 0, & r > a \end{cases}$$

- The general solution to the radial Schrödinger equation is given by

$$\chi_l(r) = \begin{cases} 0, & r \leq a \\ A_l[\hat{j}_l(kr)\cos\delta_l + \hat{n}_l(kr)\sin\delta_l], & r > a \end{cases}$$

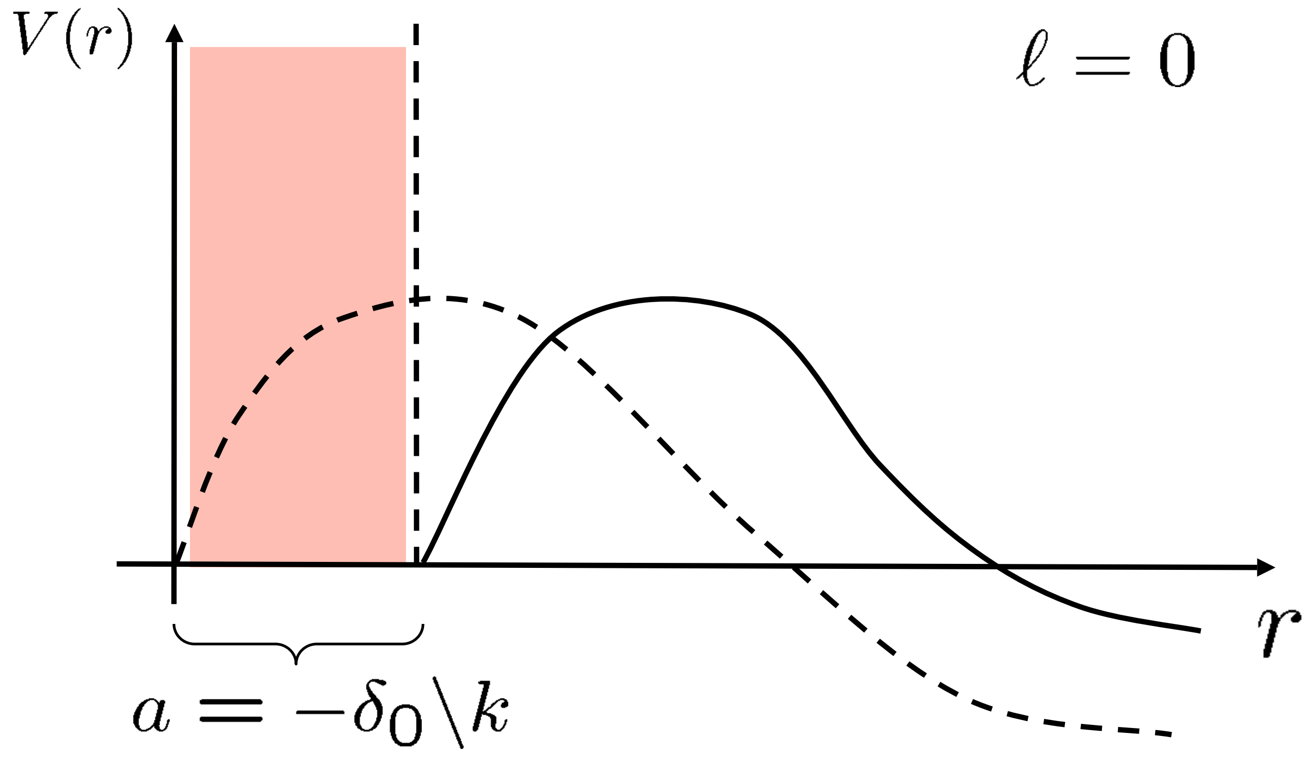
- Imposing continutity, we obtain $\chi_l(a) = 0$,

$$\Rightarrow \tan\delta_l(k) = -\frac{\hat{j}_l(ka)}{\hat{n}_l(ka)}$$



- For s-wave scattering, taking $ka \ll 1$, we obtain

$$\delta_0(k) = -\frac{\sin(ka)}{\cos(ka)} = -ka$$



- In general at low energies,

$$\delta_l(k) = -\frac{\hat{j}_l(ka)}{\hat{n}_l(ka)} = \frac{(ka)^{l+1}}{(2l+1)!!}\frac{1}{(ka)^{-l}(2l-1)!!} \sim (ka)^{2l+1}$$

from which the dominance of s-wave scattering is clear.

- Note that as $a \to 0$, $\delta_l \to 0$, and thus in the limit of a zero range delta function (in 3D), the scattering potential becomes transparent.

$$\frac{d^2\chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2m_r}{\hbar^2}[E - V(r)]\chi_{kl} = 0$$

Low-Energy Scattering

- By matching the phase shifts δ_l from the solutions to the radial Schrödinger equation with the

$$f(k,\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k\cot\delta_l - ik} P_l(\cos\theta)$$

- Contribution of higher partial waves is important at high incident energies, but for a short range potential, $\delta_l \propto k^{2l+1}$, and contributions to the scattering amplitude approach zero as k^l when $k \to 0$. This is a result of the centrifugal barrier in the radial Schrödinger equation.
- Hence, at low energies (typically $T < 100\mu$K), the scattering for distinguishable particles or identical Bosons is entirely dominated by contributions from s-wave, $l = 0$. (For Fermions, it is dominated by p-wave, $l = 1$).

$$f(k,\theta) \approx \frac{1}{k\cot\delta_0 - ik}$$

- At sufficiently low energies, the s-wave phase shift can be expanded in powers of k. This effective-range expansion is given by

$$k\cot\delta_0(k) = -1/a + r_b k^2/2 - P_s k^4/4 + ...$$

where $r \sim b$ for a Van der Waals potential, and a is called the scattering length.

$$f(k,\theta) \approx \frac{1}{k\cot\delta_0 - ik}$$

$$k\cot\delta_0(k) = -1/a + r_b k^2/2 - P_s k^4/4 + ...$$

- For small k, we thus write $f(k,\theta)$ as

$$f\,(k) = \frac{1}{-1/a - ik + r_b k^2/2 + ...}$$

- As $k \to 0$, $f(k) \to -a$.
- Note that in this limit,

$$a \approx -\frac{1}{k\cot\delta_0(k)}$$

diverging scattering length, $a \to \pm\infty$ can thus be understood in terms of a phase shift that becomes close to $\pm\pi/2$.

The Zero-Range Pseudopotential

- We see at low energies that the description of the scattering process reduces to a single parameter. Thus, we can introduce a pseudopotential if it produces these same low energy scattering properties.
- The pseudopotential with only the one necessary parameter is the zero-range pseudopotential, originally used by Fermi.

$$\langle \mathbf{r} | \, V(\mathbf{r}) \, | \psi(\mathbf{r}) \rangle = g \, \delta(\mathbf{r}) \left[\frac{\partial}{\partial r} (r \, \psi(\mathbf{r})) \right]_{r=0}$$

with

$$g = \frac{2\pi\hbar^2 a}{m_r} = \frac{4\pi\hbar^2 a}{m}$$

- The effect of regularisation here is to remove any part of the wavefunction that diverges as $1/r$. Any part of the wavefunction that does not diverge as $1/r$ is unaffected by regularisation.
- Note that if we took only a δ-function, then the potential would give rise to no scattering at all in three dimensions, as can be seen from a hard sphere in the limit $b \to 0$.
- The regularisation comes from the need to introduce the appropriate boundary conditions for $r \to \infty$.

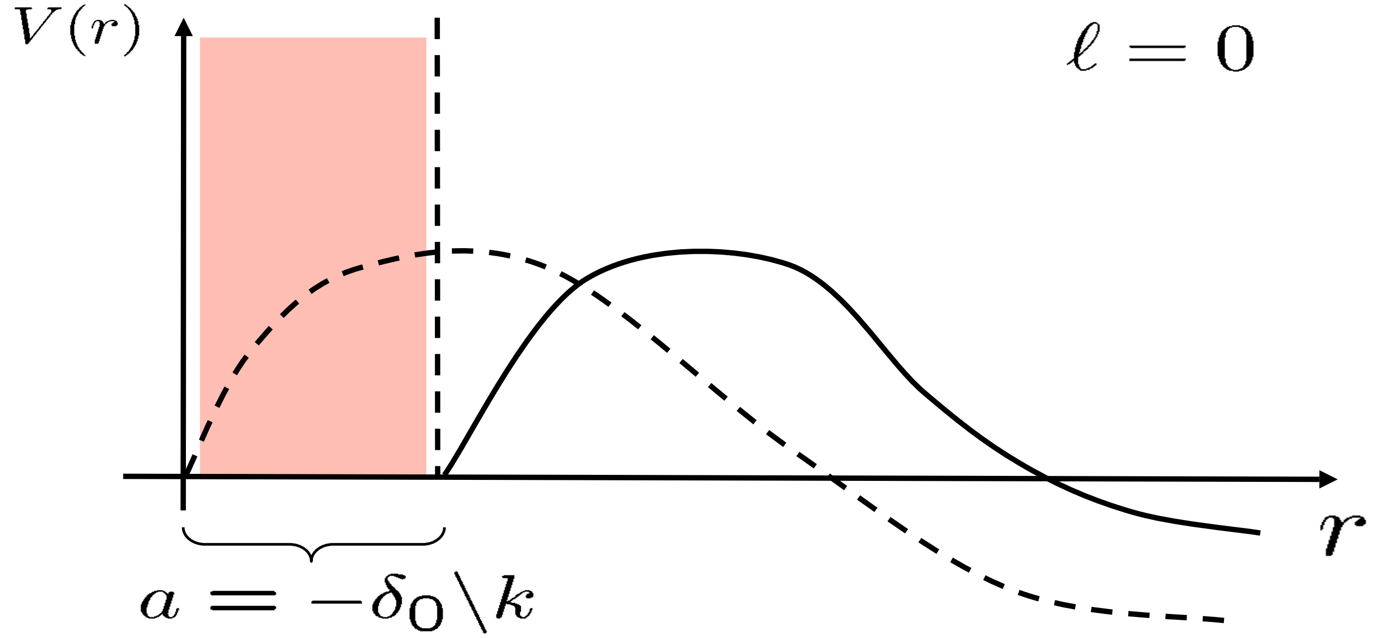
Origin of the zero-range pseudopotential

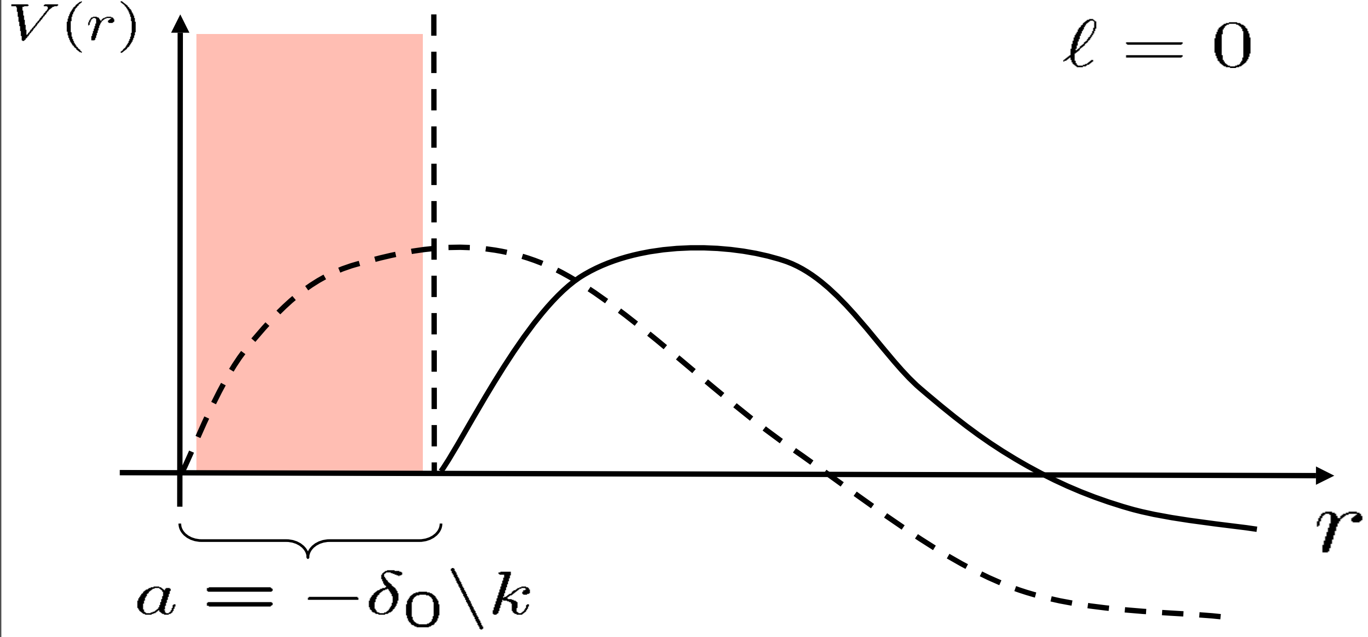
- The regularisation operator comes from the inclusion of scattering boundary conditions, as can be clearly seen in the case of the hard sphere potential (see Huang, Statistical mechanics, pp. 231-238)
- We consider again the hard sphere potential,

$$V(r) = \begin{cases} \infty, & r > a \\ 0, & r < a \end{cases}$$

for which we would like to solve the Schrödinger equation

$$\frac{\hbar^2}{2m_r}(\nabla^2 + k^2)\,\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r})$$





$\ell = 0$

$$\frac{\hbar^2}{2m_r}(\nabla^2 + k^2)\,\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r})$$

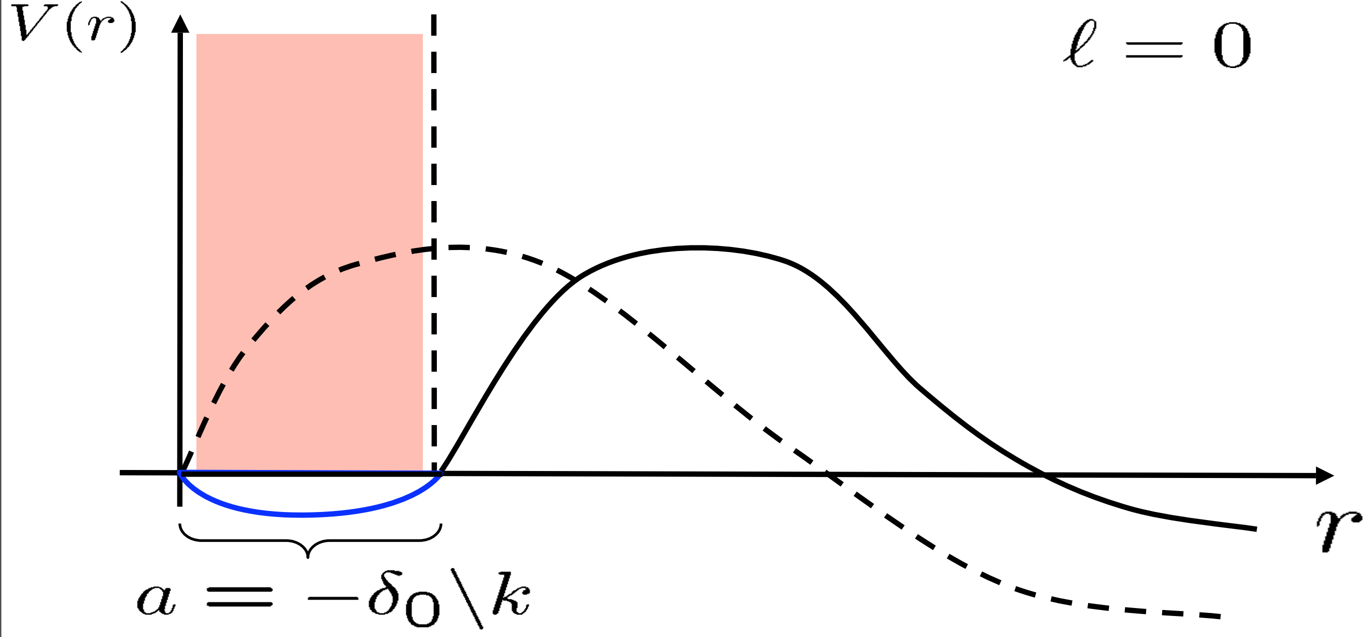
$$V(r) = \begin{cases} \infty, & r > a \\ 0, & r < a \end{cases}$$

- In the limit $k \to 0$, this reduces to

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = 0 \quad r > a$$
$$\psi(r) = 0, \qquad r < a$$

so that

$$\psi(r) = \begin{cases} C\left(1 - \frac{a}{r}\right), & r > a \\ 0, & r < a \end{cases}$$



$\ell = 0$

$$\frac{\hbar^2}{2m_r}(\nabla^2 + k^2)\,\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r})$$

$$\psi(r) = \begin{cases} C\left(1 - \frac{a}{r}\right), & r > a \\ 0, & r < a \end{cases}$$

- If we define an extended wavefunction, so that

$$(\nabla^2 + k^2)\,\psi_{ex}(\mathbf{r}) = 0$$

everywhere except at $r = 0$, with boundary condition

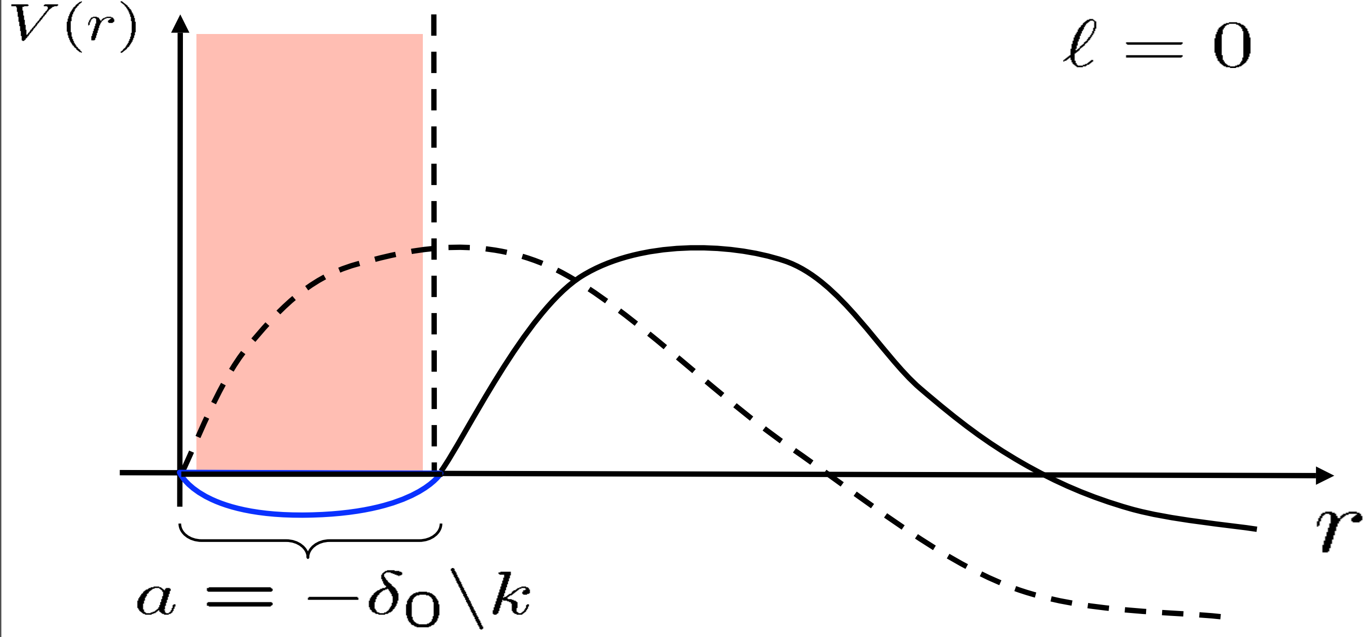
$$\psi_{ex}(a) = 0$$

then, for $k \to 0$ we obtain in the limit $r \to 0$

$$\psi_{ex}(r) \to C_0\left(1 - \frac{a}{r}\right)$$

- C_0 depends on the boundary condition at $r \to \infty$, but we can avoid using this boundary condition explicitly if we choose

$$C_0 = \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$



$\ell = 0$

$$\frac{\hbar^2}{2m_r}(\nabla^2 + k^2)\,\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r})$$

$$\psi(r) = \begin{cases} C\left(1 - \frac{a}{r}\right), & r > a \\ 0, & r < a \end{cases}$$

$$\psi_{ex}(r) \to C_0\left(1 - \frac{a}{r}\right) \qquad C_0 = \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$

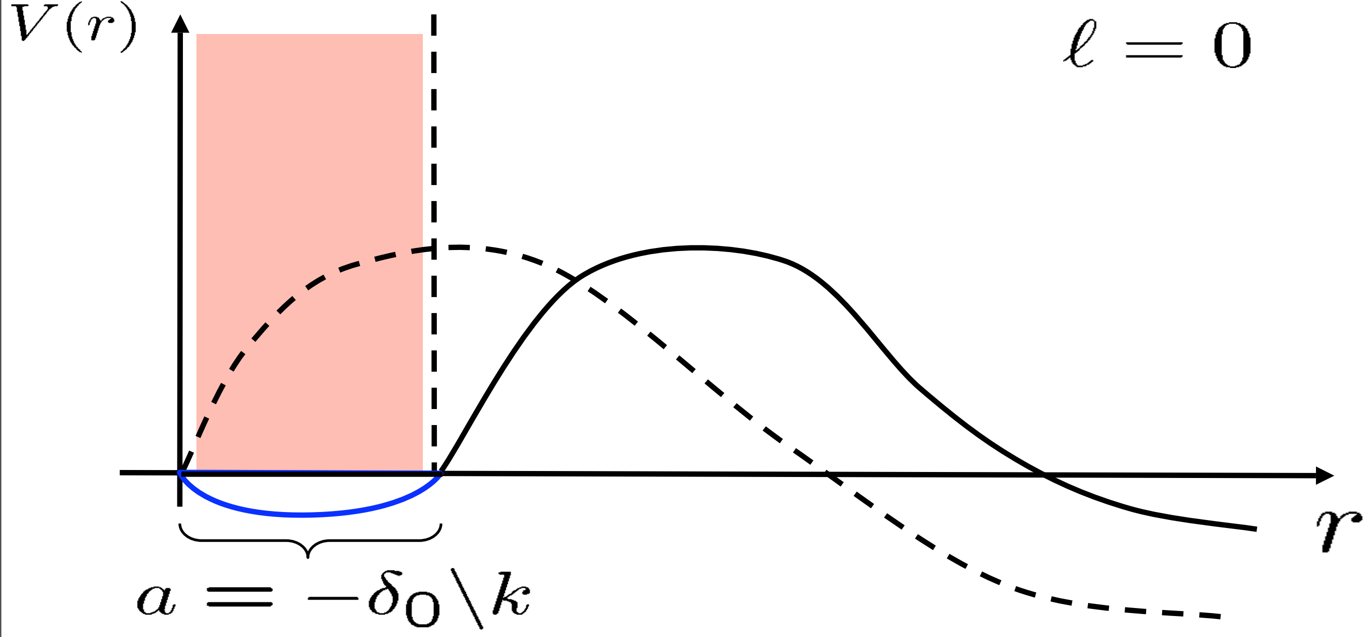
- We can then eliminate the boundary condition $\psi_{ex}(a) = 0$ by examining the behaviour of $\psi_{ex}(r)$ as $r \to 0$.

- Remembering that the Green's function for the 3D Laplacian is the function $1/r$,

$$\nabla^2 \frac{1}{r} = 4\pi\delta(\mathbf{r})$$

we can then make the replacement

$$\nabla^2\psi_{ex}(r) \to 4\pi a\delta(\mathbf{r})C_0 = 4\pi a\delta(\mathbf{r})\left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$



$$\ell = 0$$

$$\frac{\hbar^2}{2m_r}\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r})$$

$$\psi(r) = \begin{cases} C\left(1 - \frac{a}{r}\right), & r > a \\ 0, & r < a \end{cases}$$

$$\nabla^2 \psi_{ex}(r) \rightarrow 4\pi a \delta(\mathbf{r}) C_0 = 4\pi a \delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$

so that the wavefunction everywhere satisfies the equation

$$\left(\nabla^2 + k^2\right)\psi_{ex}(\mathbf{r}) = 4\pi a \delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$

or

$$\frac{\hbar^2}{2m_r}\left(\nabla^2 + k^2\right)\psi_{ex}(\mathbf{r}) = \frac{2\pi\hbar^2 a}{m_r}\,\delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$$

$$\langle \mathbf{r}|\,V(\mathbf{r})\,|\psi(\mathbf{r})\rangle = g\,\delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$$

Scattering properties of the zero-range pseudopotential

- We can compute the resulting outgoing state exactly using this potential. Writing $C_\psi = \left[\frac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$, we obtain

$$\langle \mathbf{r}|\,V(\mathbf{r})\,|\psi(\mathbf{r})\rangle = g\,\delta(\mathbf{r})\left[\frac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$$

$$\begin{aligned} f(\mathbf{k},\mathbf{k}') &= -\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i\mathbf{k}'.\mathbf{r}'}\ V(\mathbf{r}')\,\psi_{\mathbf{k}}^{(+)}(\mathbf{r}') \\ &= -g\frac{2m_r}{4\pi\hbar^2}\int d\mathbf{r}'\ \mathrm{e}^{-i\mathbf{k}'.\mathbf{r}'}\ \delta(\mathbf{r}')\ \left[\frac{\partial}{\partial r}(r\ \psi_{\mathbf{k}}^{(+)}(\mathbf{r}))\right]_{r=0} \\ &= -aC_{\psi^+} \end{aligned}$$

as $g = 4\pi\hbar^2 a/m = 2\pi\hbar^2 a/m_r$, so

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \mathrm{e}^{\mathbf{ik}.\mathbf{r}} - aC_{\psi^+}\frac{\mathrm{e}^{ikr}}{r}$$

thus,

$$\begin{aligned} r\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= r\mathrm{e}^{\mathbf{ik}.\mathbf{r}} - raC_{\psi^+}\frac{\mathrm{e}^{ikr}}{r} \\ \left[\frac{\partial}{\partial r}(r\ \psi_{\mathbf{k}}^{(+)}(\mathbf{r}))\right]_{r=0} &= \left[\frac{\partial}{\partial r}\left(r\mathrm{e}^{\mathbf{ik}.\mathbf{r}} - aC_{\psi^+}e^{ikr}\right)\right]_{r=0} \end{aligned}$$

$$\begin{aligned} C_{\psi^+} &= \left[\mathrm{e}^{\mathbf{ik}.\mathbf{r}} + ikr\mathrm{e}^{\mathbf{ik}.\mathbf{r}} - ikaC_{\psi^+}e^{ikr}\right]_{r=0} \\ C_{\psi^+} &= 1 - ikaC_{\psi^+} \end{aligned}$$

$$C_{\psi^+} = \frac{1}{1+ika}$$

$$f(\mathbf{k},\mathbf{k}') = -\frac{a}{1+ika} = \frac{1}{-1/a - ik}$$

$$C_{\psi^+} = \frac{1}{1+ika}$$

so that

$$f(\mathbf{k},\mathbf{k}') = -\frac{a}{1+ika} = \frac{1}{-1/a - ik}$$

which is the correct s-wave scattering amplitude that we obtained previously.

- Thus, we can describe scattering properties by replacing $V(r)$ with this pseudopotential.
- This is valid whenever s-wave scattering dominates, and our scattering amplitude,

$$f(k) = \frac{1}{-1/a - ik + r_b k^2/2 + \ldots} \approx \frac{1}{-1/a - ik}.$$

  Thus, the pseudopotential is valid in the limit where $kb \ll 1$. It is **not** required that $ka \ll 1$.
- Therefore, the pseudopotential may be used near a Feshbach resonance, where a diverges, but b remains constant.

Zero-Range Pseudopotential and the Born Series

- The requirement for the use of the Born approximation to be valid with the pseudopotential (as is required for mean-field theories to be used) is, indeed $ka \ll 1$:
- The Born expansion reduces to iterations of the equation

$$C_{\psi^+} = 1 - ikaC_{\psi^+},$$

in order to specify the corresponding scattering states,

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - aC_{\psi^+}\frac{e^{ikr}}{r}.$$

The Born approximation is given by the first order iteration, i.e.,

$$C_1 = 1 - ikaC_0 = 1.$$

Similarly, higher order approximations are given by:

$$C_2 = 1 - ikaC_1 = 1 - ika$$
$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2$$

and the Born expansion is a geometrical series of the exact result $C_{\psi^+} = 1/(1+ika)$ in powers of ika.

$$\langle \mathbf{r}|\, V(\mathbf{r})\, |\psi(\mathbf{r})\rangle = g\,\delta(\mathbf{r}) \left[\frac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \mathrm{e}^{\mathbf{ik.r}} - aC_{\psi^+}\frac{\mathrm{e}^{ikr}}{r}$$

$$C_\psi = \left[\tfrac{\partial}{\partial r}(r\,\psi(\mathbf{r}))\right]_{r=0}$$

$$C_1 = 1 - ikaC_0 = 1.$$

$$C_2 = 1 - ikaC_1 = 1 - ika$$

$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2$$

- The Born approximation is thus valid when the first order result is a small correction to the zeroth order result, which requires

$$k|a| \ll 1.$$

  For the scattering state, we thus require

$$r \gg a.$$

- Substituting the Pseudopotential for $V(\mathbf{r})$in the many body Hamiltonian for the case where the Born approximation is valid (and thus the regularisation in the pseudopotential gives the constant 1), we thus obtain from

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d^3r \int d^3r'\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r}')\, V(\mathbf{r}'-\mathbf{r})\, \hat{\psi}(\mathbf{r}')\, \hat{\psi}(\mathbf{r})$$

$$\hat{H} = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{g}{2}\int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}(\mathbf{r})\, \hat{\psi}(\mathbf{r})$$

Bound states of the zero-range pseudopotential

- For $a < 0$ the zero-range pseudopotential has no bound states.
- For $a > 0$, there exists exactly one bound state,

$$\psi_{bound}(\vec{r}) = \frac{1}{\sqrt{2\pi a}} \frac{e^{-r/a}}{r}.$$

  with energy

$$E_{bound} = -\frac{\hbar^2}{ma^2}.$$

- This is counter-intuitive, and the opposite result to that found for a delta function potential in 1D (where a bound state exists only for $a < 0$).
- Despite this fact, the potential is indeed repulsive for $a > 0$, and attractive for $a < 0$.
- This paradox arises from the regularising operator, which indeed makes the pseudo-potential qualitatively different from a delta potential (reminder: a delta potential in 3D does not give rise to scattering).

Summary: Many-body Hamiltonian

- The many-body Hamiltonian for the dilute, weakly interacting Bose gas may be written in terms of bosonic operators, which obey

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

as

$$\hat{H} \approx \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{g}{2}\int d^3r\;\; \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})\; \hat{\psi}(\mathbf{r})\, \hat{\psi}(\mathbf{r})$$

with $g = \frac{4\pi\hbar^2 a_s}{m}$, where a_s is the scattering length.

- This is valid under the assumptions:
  - The gas is sufficiently dilute that:
    * Only two-body interactions are important
    * We can treat the composite atoms as Bosons
  - The energy/temperature are sufficiently small that two-body scattering reduces to s-wave processes, parameterised by the scattering length.
  - That the scattering length a_s is sufficiently small that we can ignore corrections to g outside the Born approximation.

- These assumptions are typically satisfied when we load atoms from a BEC into an optical lattice. Thus, the same second-quantised Hamiltonian is valid.