S-wave scattering by central potentials in spherical and cubic boxes and contact pseudo potential

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Motivation

Simulations on lattice
In cubic boxes with periodic boundary conditions:
S-wave scattering of two particles with short range central interactions → eigen-energies, ...

Scattering theory

\[-\frac{k}{4\pi} \cot \delta(k) = \frac{1}{L^3} \sum_{|\mathbf{p}|<\Lambda} \frac{1}{p^2 - k^2} - \frac{\Lambda}{4\pi},\]

with \(\delta\) the s-wave phase shift, the incoming energy \(E = k^2/m\),
\(\mathbf{p} = \{p_x, p_y, p_z\} = \{2\pi l_x/L, 2\pi l_y/L, 2\pi l_z/L\}\), \(\Lambda\) is the momentum cutoff (\(\hbar = 1\)).
However, in spherical boxes with hard wall BCs \(\Delta k R = -\delta\).

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Motivation

Contact pseudo potential:

\[ V_{\text{eff}}(r) = \frac{4\pi a_s}{m} \delta(r), \]  \hspace{1cm} (2)

with \( a_s \) s-wave scattering length defined as

\[ a_s = \lim_{k \to 0^+} \left( -\frac{\tan \delta(k)}{k} \right). \]  \hspace{1cm} (3)

How is it derived in cubic boxes?
Scattering in spherical boxes \(^2\)

\[
\Delta k_\nu R = (k'_\nu - k_\nu) R = -\delta.
\]

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

Free s-wave:

\[
\psi_\nu(r) = \frac{1}{\sqrt{2\pi R}} \frac{\sin(k_\nu r)}{r}, \quad E_\nu = \frac{k_\nu^2}{m}
\]

With potential,

\[
\psi'_\nu(r) = \frac{1}{\sqrt{2\pi R}} \frac{\sin(k'_\nu r + \delta)}{r}, \text{ for } r > r_0
\]

\[
k'_\nu R + \delta = \nu\pi
\]

We can continue to calculate the energy change to each eigenstate

\[
\Delta E_\nu = \frac{k_\nu^{'2} - k_\nu^2}{m} = - \frac{\delta(2\nu\pi - \delta)}{mR^2} \quad \left( \lim_{k \to 0^+} \delta(k) = -ka_s \right)
\]

\[
= \frac{2\nu\pi k_\nu a_s}{mR^2}
\]

\[
= \frac{4\pi a_s}{m} |\phi_\nu(0)|^2
\]

\[
= \int d\mathbf{r} \phi_\nu^*(\mathbf{r}) V_{\text{eff}}(\mathbf{r}) \phi_\nu(\mathbf{r})
\]

with

\[
V_{\text{eff}}(\mathbf{r}) = \frac{4\pi a_s}{m} \delta(\mathbf{r})
\]
Scattering in cubic boxes

\[ [-\nabla^2 + V(r)]\psi(r) = E\psi(r) \]

Free states are simply

\[ \phi_p(r) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{p} \cdot \mathbf{r}} \]

\[ p = \{2\pi l_x/L, 2\pi l_y/L, 2\pi l_z/L\} \]

Subspaces of states with same energy,

\[ \Gamma_k = \{p|p^2 = k^2\} \],

\[ D_k \] the number elements in \( \Gamma_k \)

Free to rotate the basises:

\[ \phi_k^s(r) = \frac{1}{\sqrt{D_k L^3}} \sum_{p \in \Gamma_k} e^{i\mathbf{p} \cdot \mathbf{r}} \]

and the rest \( D_k - 1 \) basis

\[ \phi_k^{\bar{s}}(r) = \sum_{p \in \Gamma_k} c_p \phi_p(r), \]

\[ \sum_{p \in \Gamma_k} c_p = 0 \]

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S-wave scattering in cubic boxes:

\[ V(r)\phi(r) \rightarrow V(r) \int \frac{d\Omega_r}{4\pi} \phi(r) \]

By iteration, we know \( \phi^s_k \) not scattered, only \( \phi^s_k \) affected.

For \( r > r_0 \),

\[ G(r; k) = \frac{1}{L^3} \sum_p \frac{e^{ip\cdot r}}{p^2 - k^2} \]

satisfies both PBCs and Schrödinger equation with \( E = k^2 / m \).

So apart from normalization,

\[ \phi^s_k(r) \rightarrow \phi'^s_k(r) = G(r; k) \]
\[ \phi^s_k(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{p}} \frac{e^{i \mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2} \]

\[ -k \frac{\cot \delta(k)}{4\pi} = \lim_{r \to 0} \left[ \frac{1}{L^3} \sum_{\mathbf{p}} \frac{e^{i \mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2} - \frac{1}{4\pi r} \right] \]

On lattice with cutoff \( \Lambda \),

\[ -k \frac{\cot \delta(k)}{4\pi} = \frac{1}{L^3} \sum_{|\mathbf{p}|<\Lambda} \frac{1}{\mathbf{p}^2 - k^2} - \frac{\Lambda}{4\pi} \]

What’s its relation with \( \Delta k R = -\delta(k) \)?
\[ \Delta k L / 2\pi = (k - k_0) L / 2\pi = \alpha_{k_0} (-\delta) \]

\[ \alpha_{k_0} = D_{k_0} / (k_0 L)^2 \]
For nonresonance, \( \lim_{k \to 0^+} \delta(k) = -k a_s \)

\[
\Delta k L/2\pi = D_{k_0}/(k_0 L)^2 (-\delta)
\]

always good.

Calculate the energy change

\[
\Delta E = (k^2 - k_0^2)/m
\]

\[
= \frac{4\pi a_s D_{k_0}}{m L^3}
\]

\[
= \frac{4\pi a_s}{m} |\phi_{k_0}^s(0)|^2
\]

where \( \phi_{k}^s(r) = \frac{1}{\sqrt{D_{k} L^3}} \sum_{p \in \Gamma_k} e^{i p \cdot r} \)

Consistent with

\[
V_{\text{eff}}(r) = \frac{4\pi a_s}{m} \delta(r)
\]