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[1]

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

with δ the s-wave phase shift, the incoming energy $E = k^2/m$, $\mathbf{p} = \{p_x, p_y, p_z\} = \{2\pi l_x/L, 2\pi l_y/L, 2\pi l_z/L\}$, Λ is the momentum cutoff ($\hbar = 1$).

However, in spherical boxes with hard wall BCs $\Delta k R = -\delta$.

[1] S.R. Beane, P.F.Bedaque, A. Parreno and M.J. Savage, Phys. Lett. B **585**, 106 (2004).

Motivation

Contact pseudo potential:

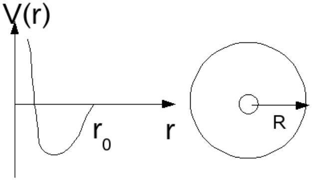
$$V_{\text{eff}}(r) = \frac{4\pi a_s}{m}\delta(\mathbf{r}), \tag{2}$$

with a_s s-wave scattering length defined as

$$a_s = \lim_{k\to 0^+} -\frac{\tan\delta(k)}{k}. \tag{3}$$

How is it derived in cubic boxes?

Scattering in spherical boxes[2]



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

Free s-wave:

$$\psi_\nu(\mathbf{r}) = \frac{1}{\sqrt{2\pi R}}\frac{\sin(k_\nu r)}{r}$$

$$k_\nu R = \nu\pi,\ E_\nu = k_\nu^2/m$$

With potential,

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

$$\psi'_\nu(\mathbf{r}) = \frac{1}{\sqrt{2\pi R}}\frac{\sin(k'_\nu r + \delta)}{r},\ \text{for r} > \text{r}_0$$

$$k'_\nu R + \delta = \nu\pi$$

[2] A.J. Leggett, *Quantum Liquids: Bose Condensation and Cooper Pairing in Condensed-Matter Systems*, Oxford.

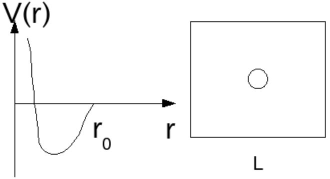
We can continue to calculate the energy change to each eigenstate

$$\begin{aligned}\Delta E_\nu =& \frac{{k'_\nu}^2 - k_\nu^2}{m} \\ =& -\frac{\delta(2\nu\pi - \delta)}{mR^2} \leftarrow \lim_{k\to 0^+}\delta(k) = -ka_s \\ =& \frac{2\nu\pi k_\nu a_s}{mR^2} \\ =& \frac{4\pi a_s}{m}|\phi_\nu(0)|^2 \\ =& \int \mathrm{d}\mathbf{r}\phi_\nu^*(\mathbf{r})V_{\text{eff}}(\mathbf{r})\phi_\nu(\mathbf{r})\end{aligned}$$

with

$$V_{\text{eff}}(\mathbf{r}) = \frac{4\pi a_s}{m}\delta(\mathbf{r}) \tag{4}$$

Scattering in cubic boxes[3]



Subspaces of states with same energy,

$\Gamma_k = \{\mathbf{p} | \mathbf{p}^2 = k^2\}$,

D_k the number elements in Γ_k

Free to rotate the basises:

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

and the rest $D_k - 1$ basis

$$\phi_k^{\bar{s}}(\mathbf{r}) = \sum_{\mathbf{p} \in \Gamma_k} c_{\mathbf{p}} \phi_{\mathbf{p}}(\mathbf{r}),$$

$$\sum_{\mathbf{p} \in \Gamma_k} c_{\mathbf{p}} = 0$$

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

Free states are simply

$$\phi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{p}\cdot\mathbf{r}}$$

$$\mathbf{p} = \{2\pi l_x/L, 2\pi l_y/L, 2\pi l_z/L\}$$

[3]M. Lüscher, Nucl. Phys. B **354**, 531 (1991).

S-wave scattering in cubic boxes:

$$V(r)\phi(\mathbf{r}) \to V(r)\int \frac{d\Omega_{\mathbf{r}}}{4\pi}\phi(\mathbf{r})$$

By iteration, we know $\phi_k^{\bar{s}}$ not scattered, only ϕ_k^s affected.

For $r > r_0$,

$$G(\mathbf{r};k) = \frac{1}{L^3}\sum_{\mathbf{p}} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2 - k^2}$$

satisfies both PBCs and Schrödinger equation with $E = k^2/m$.

So apart from normalization,

$$\phi_k^s(\mathbf{r}) \to \phi_k'^s(\mathbf{r}) = G(\mathbf{r};k)$$

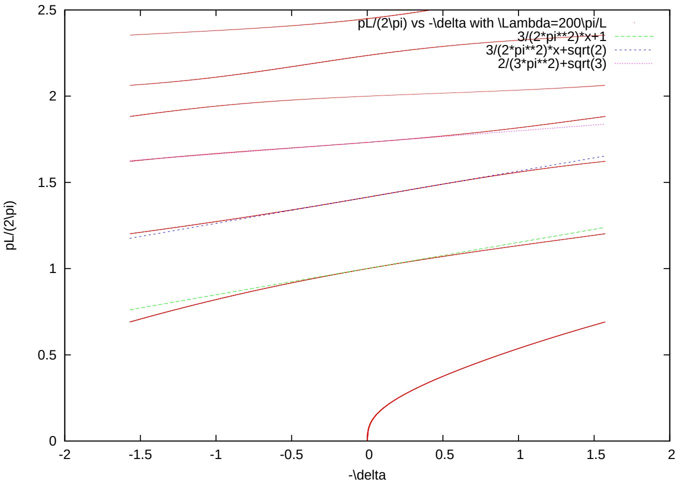
$$\phi_k'^s(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{p}} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2 - k^2}$$

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

On lattice with cutoff Λ,

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

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, $\lim_{k\to 0^+}\delta(k) = -ka_s$

$$\Delta kL/2\pi = D_{k_0}/(k_0L)^2(-\delta)$$

always good.
Calculate the energy change

$$\begin{aligned}\Delta E =& (k^2 - k_0^2)/m \\ =& \frac{4\pi a_s D_{k_0}}{mL^3} \\ =& \frac{4\pi a_s}{m}|\phi^s_{k_0}(0)|^2\end{aligned}$$

where $\phi^s_k(\mathbf{r}) = \frac{1}{\sqrt{D_k L^3}}\sum_{\mathbf{p}\in\Gamma_k} e^{i\mathbf{p}\cdot\mathbf{r}}$
Consistent with

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