Effective interaction for Bose-Einstein condensates and Rydberg atoms

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1 Introduction

- In the theory of ultracold gases, interactions are generally described by

$$V(\vec r) = \frac{2\pi\hbar^2 a}{\mu}\delta(\vec r) \quad (1)$$

where $a = -\lim_{k\to 0}[\delta_0(k)/k]$ is the scattering length and $\delta_0(k)$ is the s-wave phase shift.

- In the limit $k|a| \ll 1$, Eq. (1) correctly determines both the asymptotic wave function and the energy shift.

- For higher scattering energies, the potential in Eq. (1) with $a(k) = -\tan\delta_0(k)/k$ produces the correct asymptotic relative wave function [1, 2] but, if used in first order perturbation theory, returns a wrong energy shift:

$$\Delta E = \frac{2\pi\hbar^2}{\mu}\left[-\frac{\tan\delta_0(E)}{k}\right]|\psi(0)|^2. \quad (2)$$

Indeed, this result predicts unphysical divergences: on general grounds, $\Delta E \propto \delta_0(E)$.

2 Energy shifts vs. phase shift

- Two non-interacting bosons in a spherical box of radius R, relative wave function:

$$\psi(r) = A\frac{\sin(k_0 r)}{r}. \quad (3)$$

- By turning on the interaction, the asymptotic wave is phase shifted

$$\psi(r) = A\frac{\sin(kr+\delta_0)}{r}. \quad (4)$$

- The boundary condition implies a wave vector shift $\delta_0 = k_0R - kR$, and

$$\Delta E = \frac{\hbar^2}{\mu}k_0\Delta k = \frac{2\pi\hbar^2}{\mu}\left(-\frac{\delta_0}{k_0}\right)|\psi(0)|^2. \quad (5)$$

3 WKB approximation

- In a slowly varying potential,

$$\psi(r) = \frac{A}{r\sqrt{p(r)}}\sin\left[\int_0^r dr'\sqrt{\frac{2\mu[E-V(r')]}{\hbar^2}}\right], \quad (6)$$

- If a short range impurity is superposed, the boundary conditions require

$$\int_0^{r_c'} dr\sqrt{\frac{2\mu[E+\Delta E-V(r)]}{\hbar^2}} + \delta_0(E+\Delta E) = (n+\alpha)\pi, \quad (7)$$

and the energy shift is again given by Eq. (5).

4 Effective range correction

- The first correction to the low-energy result $\delta_0 = -ka$ is

$$k\cot\delta_0 = -\frac{1}{a} + \frac{1}{2}r_e k^2 + o\left(k^2\right), \quad (8)$$

Since $\delta_0 \sim \tan\delta_0 - \tan^3\delta_0/3$,

$$\Delta E = \frac{2\pi\hbar^2}{\mu}\left(-\frac{\delta_0}{k}\right) = \frac{2\pi\hbar^2 a}{\mu}\left(1 - g_2k^2\right) \quad (9)$$

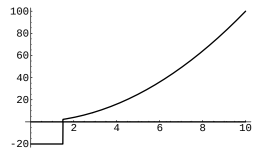
with $g_2 = a^2/3 - ar_e/2$.

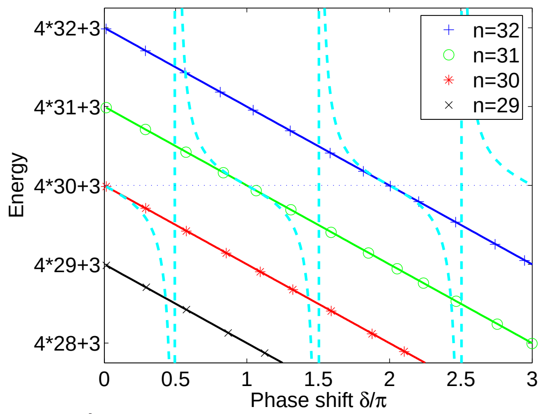
- For hard-spheres $a = R$, $r_e = 2R/3$ and correctly $g_2 = 0$ since $\delta(k)/k = -R$.

5 Comparison with other theories

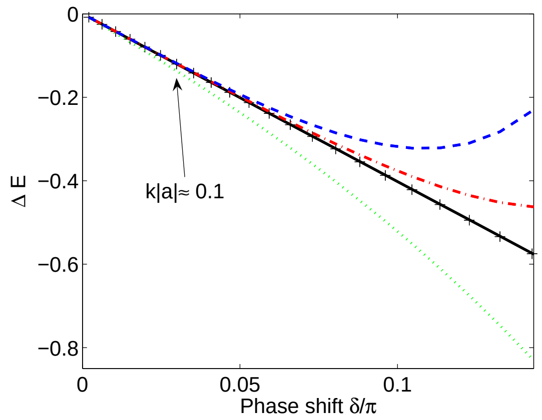
- [3, 4]: choosing V such that $\Delta E \propto \tan\delta$, $g_2 = -ar_e/2$.
- [5]: choosing V such that $\Delta E \propto \mathrm{Re}(e^{i\delta}\sin\delta) = \sin\delta\cos\delta$, $g_2 = a^2 - ar_e/2$.
- In [6] it is found a potential that reproduces the correct energy shifts in all partial waves.

6 Harmonic potential + square well impurity





Energy levels: exact values (symbols) compared to the results of Eq. (5). The dashed line is the energy shift given by Eq. (2). [y-axis in units of $\hbar\omega/2$, core width: $2a_{\text{ho}}$]



Energy shift for the $n=1$ level: exact results (+) compared with $\Delta E = 2\pi\hbar^2[\ldots]|\psi(0)|^2/\mu$, where $[\ldots]$ is replaced by either the exact $-\delta_0/k$ (solid), or by $a\,(1-g_2k^2)$ with

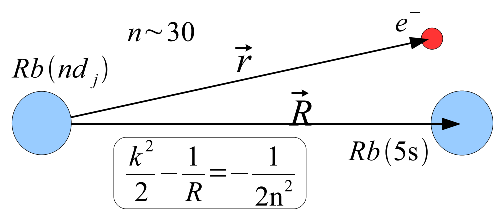
- zero-energy result $g_2 = 0$ (scattering length approx., dotted)
- our effective range correction $g_2 = \frac{a^2}{3} - \frac{ar_e}{2}$ (dashed-dotted)
- the result by [5], i.e. $g_2 = a^2 - \frac{ar_e}{2}$ (dashed).

[y-axis in units of $\hbar\omega/2$, core width: $L = 0.25a_{\text{ho}}$]

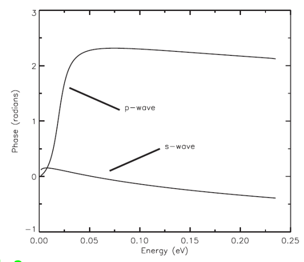
7 Collisions between Rydberg and neutral atoms

In the literature [3, 4, 7]:

- $U_s(\vec R) = -\frac{2\pi\hbar^2}{\mu}\frac{\tan\delta_0(k)}{k}|\psi_{nd0}(\vec R)|^2$.
- $U_p(\vec R) = -\frac{6\pi\hbar^2}{\mu}\frac{\tan\delta_1(k)}{k^3}|\nabla\psi_{nd0}(\vec R)|^2$.



Presence of a p-wave resonance for $R \sim 700$ a.u.:



Open question:

- Possible to find an easy answer for non-separable potenials?

References

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