Lectures on quantum gases

Lecture 3

# Elastic Collision Phenomena in Quantum Gases

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## Where do we stand?

- 1. We identified the phase shift as the central quantity for scattering
- 2. We determined the scattering amplitude (4 expressions for  $f_l$ )
- 3. We derived the differential and total cross sections
- 4. We identified the role of quantum statistics
- 5. We studied the phase shift for hard spheres
- 6. We studied the phase shift for spherical square wells
- 7. We defined the scattering length
- 8. We studied its dependence on the well parameter



# s-wave scattering length a

well parameter

$$a = r_0 \left(1 - \tan \gamma / \gamma\right)$$
  $\gamma \equiv \kappa_0 r_0$ 



# collisional significance of scattering length

$$f_{l} = \frac{1}{2ik}(e^{2i\eta_{l}} - 1) \qquad (a) \qquad \eta_{0} = -ka$$

$$= k^{-1}e^{i\eta_{l}}\sin\eta_{l} \qquad (b) \rightarrow f_{l} = \frac{1}{k}e^{i\eta_{l}}\sin\eta_{l} \qquad \int_{k \to 0}^{\eta_{0}} \frac{1}{k} \int_{k \to 0}^{\infty} \frac{1}{k} \int_$$

#### Bosons (even partial waves): s-wave scattering

$$\sigma = \frac{8\pi}{k^2} \sum_{l=\text{even}} (2l+1) \sin^2 \eta_l \quad \longrightarrow \sigma_0 = \frac{8\pi}{k^2} \sin^2 \eta_0 \quad \longrightarrow \sigma_0 = \frac{8\pi}{k^2} \sin^2 ka$$

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$$\sigma_0 = 8\pi a^2$$

## collisions of ultracold atoms



## elastic cross section for identical bosons



divergence of the scattering length

What is happening?

## universal behavior near threshold

### spherical square well for l = 0 and $\varepsilon < 0$

# spherical square well for l = 0 and $\varepsilon < 0$

$$\begin{array}{c|c}
\varepsilon & \chi_{0}^{\prime\prime} + \begin{bmatrix} k^{2} - U(r) \end{bmatrix} \chi_{0} = 0 \\
K_{+}^{2} & K_{+}^{2} = k^{2} + \kappa_{0}^{2}; \\
& & \chi_{0}^{2} = -\kappa^{2} & \chi_{0}^{\prime\prime} = 0 \\
\hline & & \chi_{0}^{2} = -\kappa^{2} & \chi_{0}^{\prime\prime} = -\kappa^{2} & \chi_{0}^$$

boundary condition:  $\chi_0(r)$  and  $\chi_0'(r)$  continuous at  $r=r_0$ 

$$r \le r_0 \qquad r > r_0$$
  
$$\chi_0'/\chi_0|_{r=r_0} = K_- \cot K_- r_0 = -\kappa \qquad \text{Bethe-Peierls boundary condition}$$

$$K_{-}^{2} = \kappa_{0}^{2} - \kappa_{0}^{2} \longrightarrow K_{-} \rightarrow \kappa_{0} \longrightarrow \chi_{0}^{\prime}/\chi_{0}|_{r=r_{0}} = \kappa_{0} \cot \kappa_{0} r_{0} = 0 \text{ for } \kappa \rightarrow 0$$

$$(\text{Conclusion: next bound state appears for } \gamma = \frac{\pi}{2} + n\pi)$$
9

# binding energy versus well parameter



#### universal behavior near threshold ${\mathcal E}$ Continuum state near threshold: $K^2_+$ $+k^2 - \varepsilon > 0$ $(k \to 0)$ $\kappa_0 \cot \kappa_0 r_0 = \frac{1}{r_0 - a} \simeq -\frac{1}{a}$ $r_0$ $K^2$ Bound state near threshold: $\varepsilon_b$ $\varepsilon < 0 \quad (\kappa \to 0) \quad \kappa_0 \cot \kappa_0 r_0 \simeq -\kappa \quad (\kappa > 0)$ $a = \frac{1}{-}$ $\kappa_0^2$ $U_0$

Universal dependence of binding energy on scattering length:

 $\rightarrow$  a > 0 for  $\kappa \rightarrow 0$ 

$$\varepsilon = -\kappa^2 = -\frac{1}{a^2} \longrightarrow \qquad E_b = -\frac{\hbar^2}{2\mu} \frac{1}{a^2}$$

# scattering length a

Continuum states (
$$\varepsilon > 0$$
):  

$$\eta_0 = -ka$$

$$\chi_0(r) = \sin(kr + \eta_0) = \sin[k(r - a)] \underset{k \to 0}{\simeq} k(r - a)$$



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# halo states

#### Bound states ( $\epsilon < 0$ ):

# $\chi_0 = A e^{-\kappa r}$ universal bound states: halo states $\kappa r_0 \ll 1$

strange molecule: large probability to find the atoms outside the classical turning point



# halo states



# significance of s-wave scattering length

We distinguish between:

(a) thermodynamic significance(b) collisional significance

Thermodynamic significance particle spherical (macroscopic) box:

(a) without interaction

$$R_0^{(0)}(k_n, r) = \sqrt{\frac{2}{R}} \frac{\sin[k_n r]}{r}$$
  $k_n = n \frac{\pi}{R}$ 

(b) with interaction

$$R_0(k'_n, r) =_{r > r_0} \sqrt{\frac{2}{R}} \frac{\sin[k'_n r + \eta_0(k'_n)]}{r} \qquad k'_n = n \frac{\pi}{R - a}$$

$$\delta E = \frac{\hbar^2}{2m} \left( k_n^{\prime 2} - k_n^2 \right) \simeq n^2 \frac{\hbar^2}{m} \frac{\pi^2}{R^3} a$$



 $\eta_0 = -k'_n a$ 

## significance of *s*-wave scattering length

$$\delta E = \frac{\hbar^2}{2m} \left( k_n^{\prime 2} - k_n^2 \right) \simeq n^2 \frac{\hbar^2}{m} \frac{\pi^2}{R^3} a$$

## significance of s-wave scattering length

 $\delta E = \frac{\hbar^2}{2m} \left( k_n'^2 - k_n^2 \right) \simeq n^2 \frac{\hbar^2}{m} \frac{\pi^2}{R^3} a \qquad \text{repulsive for } a > 0$  attractive for a < 0 $\chi_0(r)$ ground state (n = 0):  $R_0(r)$ n(r) $n_0$ R R R  $1 = \int \left|\psi_0(\mathbf{r})\right|^2 d\mathbf{r} = \int n(\mathbf{r}) d\mathbf{r} = n_0 \int \frac{n(\mathbf{r})}{n_0} d\mathbf{r}$  $V_e \longrightarrow V_e \equiv \frac{N}{n_e} = \frac{2}{\pi}R^3$  $\delta E = \frac{4\pi\hbar^2}{m} \frac{a}{V_e}$ 

## pedestrian view on chemical potential

$$\delta E = \frac{4\pi\hbar^2}{m} \frac{a}{V_e} \longrightarrow E = \delta E \frac{N(N-1)}{2} \longrightarrow \left[ E \simeq \frac{2\pi\hbar^2}{m} a \frac{N^2}{V_e} \right]$$

Chemical potential at T = 0:

$$\mu = \frac{\partial E}{\partial N} = \frac{4\pi\hbar^2}{m} a n_0$$
$$\mu = g_0 n_0$$
$$g_0 = \frac{4\pi\hbar^2}{m} a$$
$$\mathcal{V}(\mathbf{r}_1 - \mathbf{r}_2) = g_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

Relative motion of interacting particles II

# flat-bottom potential

effective range -  $r_e$ 

# effective range $r_e$

We now analyze the energy dependence of the phase shift

$$\eta_0(k) = -kr_0 + \arctan \frac{k}{K_+ \cot K_+ r_0}$$
  
"regular" "resonant"  

$$\tan(\alpha + \beta) = \frac{\tan \alpha + \tan \beta}{1 - \tan \alpha \tan \beta}$$
  

$$\tan x = x + \frac{1}{3}x^3 + \dots = x(1 + \frac{1}{3}x^2 + \dots)$$

evaluate phase shift:

$$kr_0 \cot \eta_0 = \frac{K_+ r_0 \cot K_+ r_0 + k^2 r_0^2 + \cdots}{1 - \left(1 + \frac{1}{3}k^2 r_0^2 + \cdots\right) K_+ r_0 \cot K_+ r_0}$$

$$K_{+}^{2} = k^{2} + \kappa_{0}^{2} \longrightarrow K_{+}r_{0} = \kappa_{0}r_{0}[1 + k^{2}/\kappa_{0}^{2}]^{1/2} = \gamma + \frac{1}{2}k^{2}r_{0}^{2}/\gamma + \cdots$$

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# effective range $r_e$

$$kr_{0} \cot \eta_{0} = -\frac{1}{1 - \tan \gamma/\gamma} + \frac{1}{2}k^{2}r_{0}^{2} \left(1 - \frac{3\left(1 - \tan \gamma/\gamma\right) + \gamma^{2}}{3\gamma^{2}\left(1 - \tan \gamma/\gamma\right)^{2}}\right) + \cdots$$

 $a = r_0 \left(1 - \tan \gamma / \gamma\right)$   $r_e : \text{ measure for energy dependence}$ of the phase shift

Effective range expansion:

$$k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2}k^2 r_e + \cdots - k \cot \eta_0 = -\frac{1}{a(k)}$$
  
Effective range:  $r_e = r_0 \left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3\gamma^2 a^2}\right)$ 

Two expansions to order  $k^2$ :

$$a \neq 0 \qquad k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2}k^2 r_0 \left( 1 - \frac{3ar_0 + \gamma^2 r_0^2}{3\gamma^2 a^2} \right) + \cdots$$
$$a \ll r_0 \qquad \frac{1}{k \cot \eta_0} = -a + \frac{1}{6}k^2 r_0^3 [1 - 3\left(\frac{a}{r_0}\right)^2 + \left(\frac{3}{\gamma^2}\right)\left(\frac{a}{r_0}\right)] + \cdots$$

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. . .

effective range 
$$r_e$$
 - special cases  
 $a \neq 0$   $k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2}k^2r_0\left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3\gamma^2 a^2}\right) + \cdots$   
 $r_e$  positive  
 $a = \pm r_0$  (regular)  $r_e = r_0\left(2/3 \mp 1/\gamma^2\right) \simeq \frac{2}{3}r_0$   
 $k \cot \eta_0 = \mp \frac{1}{r_0} + \frac{1}{3}k^2r_0 + \cdots$   
 $kr_0 \ll 1 \longrightarrow k$  dependence unimportant  
positive  
 $|a| \gg r_0$  (anomalously large)  $r_e \neq r_0$   
 $k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2}k^2r_0 + \cdots$   
 $\rightarrow \text{ strong } k$  dependence of  $a(k)$ 

effective range 
$$r_e$$
 – special cases  
 $a \ll r_0$   $\frac{1}{k \cot \eta_0} = \checkmark a + \frac{1}{6}k^2 r_0^3 [1 - 3(a/r_0)^2 + (3/\gamma^2)(a/r_0)] + \cdots$ 

a = 0 (anomalously small)  $k \cot \eta_0 = -\frac{1}{a(k)} = \frac{6}{k^2 r_0^3} + \cdots$   $a(k) = -\frac{1}{6}k^2 r_0^3$  $kr_0 \ll 1 \longrightarrow k$  dependence large but a always small

Conclusions for 'open channel' potentials: effective range always positive - important only for  $|a| \gg r_0$ 

## examples

ultracold atom collisions:

<sup>133</sup> Cs  4,4>	$a = 2400 a_0$	$r_0 = 100 a_0$
<sup>85</sup> Rb  3,3>	$a = -369 a_0$	$r_0 = 83 a_0$
<sup>88</sup> Sr	$a = -2 a_0$	
<sup>1</sup> H  1,1>	$a = 1.22 a_0$	$r_e = 348 \ a_0$

#### 2 hadron collisions at MeV energies:

s-wave regime  $(kr_0 \ll 1)$ :

 $r_0$  is 6 orders of magnitude smaller

proton (uud) I=1/2

**neutron (udd)** I = 1/2 k can be 6 orders of magnitude larger

deuteronI = 1bound statea > 0a = 5.41 fm $r_e = 1.75$  fmI = 0virtual statea < 0a = -2.38 fm $r_e = 2.67$  fm

# Relative motion of interacting particles II

- 1. We explored the scattering length
- 2. We studied its dependence on the well parameter
- 3. We demonstrated elastic scattering with Rb-87
- 4. We found resonant enhancement near the bound state threshold
- 5. We found universal behavior near the bound state threshold
- 6. We defined halo states and zero-range potentials
- 7. We analyzed the energy dependence of the scattering length
- 8. We introduced the effective range  $r_e$
- 9. We analyzed when the effective range is important
- 10. We discussed anomalously large and small scattering lengths
- 11. We discussed some examples