Three-body scattering hypervolume of soft-sphere boson

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Outline

- Low-energy 2-body and 3-body collisions
- Definition of three-body scattering hypervolume D
- Calculation of D for soft-sphere bosons
- Extensions

Low-energy 2-body collisions

- 2 particles colliding at low energies in s-wave

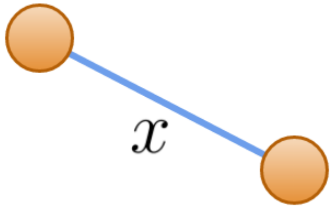
$$\psi = \phi + Ef + E^2 g + E^3 h + \cdots$$

$$H_{2b}\phi = 0, \quad H_{2b} f = \phi, \quad H_{2b} g = f \ldots$$

- Wave function at $E = 0$ outside the range of interaction

$$\phi(x) = 1 - \frac{a}{x}$$

a: two-body scattering length

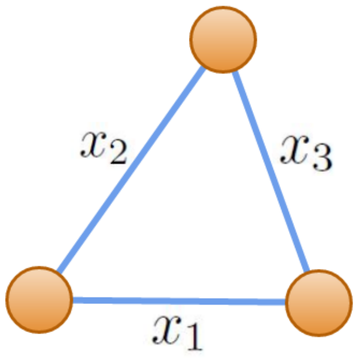


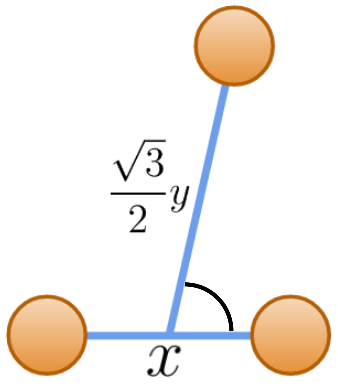
Low-energy 3-body collisions

- Three identical bosons with short-range interactions at $E = 0$

$$\left[-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_3^2 + V(x_1) + V(x_2) + V(x_3) + V_3(x_1, x_2, x_3)\right]\phi = 0$$

- Zero total momentum and zero total orbital angular momentum
- Wave function depends on three pairwise distances



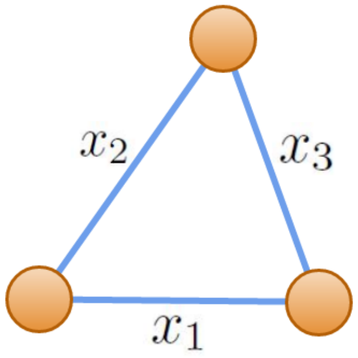


Asymptotic expansions at large distances

- 111-expansion

  fix shape, let $x_1, x_2, x_3 \to \infty$ simultaneously

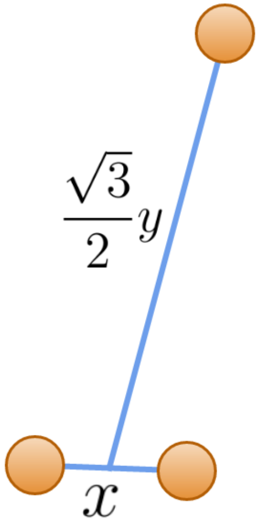
  series of $1/\rho$, hyperradius $\rho = \sqrt{\frac{x_1^2+x_2^2+x_3^2}{2}}$



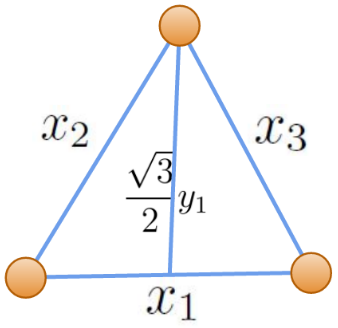
- 21-expansion

  fix x, at $y \to \infty$

  series of $1/y$



111-expansion



$$\phi^{(111)} = 1 + \Big(\sum_{i=1}^{3} -\frac{a}{x_i} + \frac{8a^2\theta_i}{\sqrt{3}\pi x_i y_i} - \frac{2wa^3}{\pi x_i \rho^2} + \frac{8\sqrt{3}wa^4(\ln\frac{e^\gamma \rho}{|a|} - 1 - \theta_i \cot 2\theta_i)}{\pi^2\rho^4}\Big) - \frac{\sqrt{3}D}{8\pi^3\rho^4} + \cdots + O(\frac{1}{\rho^8})$$

[S. Tan PRA **78**, 013636 (2008)]

- Hyperradius $\rho = \sqrt{\frac{x_1^2+x_2^2+x_3^2}{2}}$, $\theta_i = \arctan\frac{y_i}{x_i}$,
  $w = \frac{4\pi}{3} - \sqrt{3}$, Euler's constant $\gamma \approx 0.577\,215\,664$
- D: three-body scattering hypervolume, [Length]^4

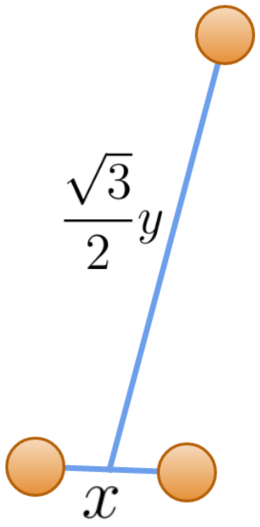
21-expansion

$$\phi^{(21)} = \Big(1 - \frac{4a}{\sqrt{3}y} + \frac{8a^2w}{3\pi y^2} - \frac{32a^3w}{3\sqrt{3}\pi y^3} + \frac{384\sqrt{3}wa^4(\ln\frac{\sqrt{3}e^\gamma y}{2|a|} - 3/2) - 16\xi_1}{9\pi^2 y^4}\Big)\phi(x) + \frac{16a^2w}{3\pi^2y^4}f(x)$$

$$+ \Big(-\frac{20a}{\sqrt{3}y^3} + \frac{640(2\pi - 3\sqrt{3})a^2}{9\pi y^4}\Big)\phi^{(d)}_{\hat{\mathbf{y}}}(\mathbf{x}) + \cdots + O(\frac{1}{y^8})$$

[S. Tan PRA **78**, 013636 (2008)]

$$\xi_1 = \frac{\sqrt{3}D}{8\pi} - 8(\sqrt{3} - \pi/3)wa^4 - \frac{3\pi w}{2}a^3 r_s$$



- 2-body s-wave: $\phi(x)$, $f(x)$, …
  $H_{2b}\phi = 0, \quad H_{2b}f = \phi$
- 2-body d-wave: $\phi^{(d)}_{\hat{\mathbf{y}}}(\mathbf{x})$, …
  $H_{2b}\phi^{(d)}_{\hat{\mathbf{y}}}(\mathbf{x}) = 0$

Applications of D

- Affect systems with $N \geq 3$ particles, at zero or finite termperatures
- Ground state energy of a dilute BEC, the nonuniversal n^2 term

$$\frac{E}{N} = 2\pi na\left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} + 8wna^3\ln(na^3) + (\frac{\pi r_s}{a} + 118.498\,920\,346)na^3\right] + \frac{1}{6}Dn^2 + o(n^2)$$

[E. Braaten & A. Nieto 1999, S. Tan 2008]

- Critical temperature
- Equation of state of Bose gases at finite temperatures
- …

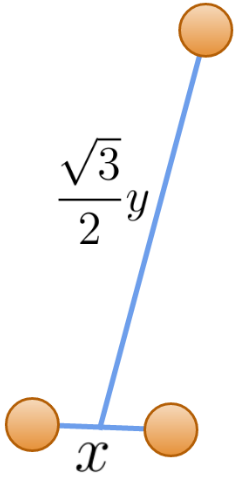
Calculation of D

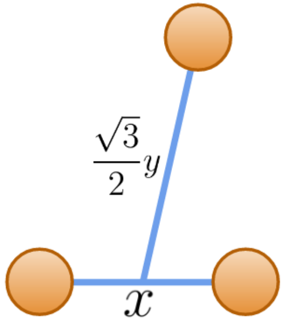
- Hard-sphere bosons, $V_{HS}(r) = \begin{cases} +\infty, r < a \\ 0, r > a \end{cases}$

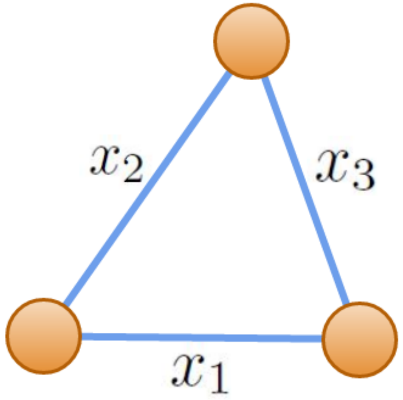
  $D_{HS} \approx 1761.5a^4$, by S. Tan 2008

- Soft-sphere bosons, $V(r) = v_0 \exp(-r^2)$

Error analysis of the two expansions at large ρ







- 21-expansion at $x \sim 1$
- Error $\sim \rho^{-8}$

- Intermediate region $x \sim \rho^{1/3}$
- Both expansions have errors $\sim \rho^{-6}$

- 111-expansion at $x_i \sim \rho$
- Error $\sim \rho^{-8}$

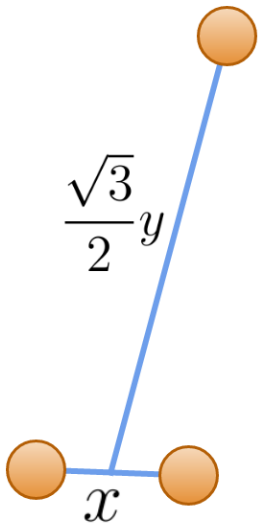
$$\rho = \frac{\sqrt{3}}{2}\sqrt{x^2 + y^2} = \sqrt{\frac{x_1^2 + x_2^2 + x_3^2}{2}}$$

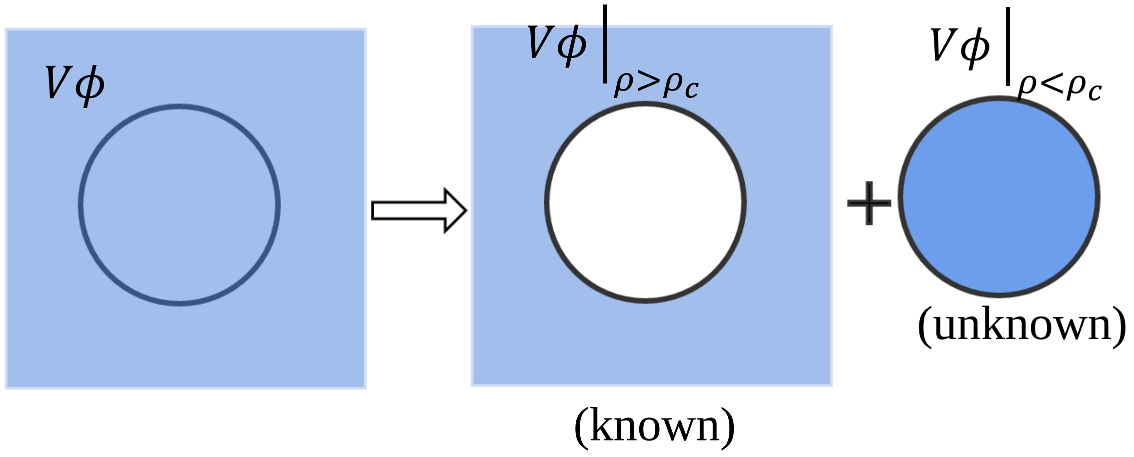
A detour, considering $V\phi$

- $V\phi$ well approximated by 21-expansion at large ρ

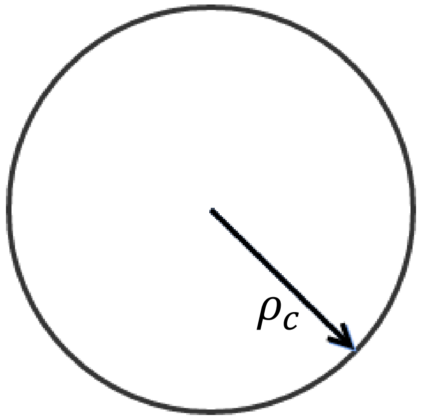
$$V\phi \approx V(x_1)\phi_1^{(21)} + V(x_2)\phi_2^{(21)} + V(x_3)\phi_3^{(21)}$$

- $V\phi$ known outside a large hypersphere $\rho > \rho_c$





Wave function at large ρ_c



- $\nabla^2\phi = V\phi$ in 6 dimensions
- Consider $V\phi$ as the source
- Divide the source into two pieces: $\rho' > \rho_c$ and $\rho' < \rho_c$

$$\begin{aligned}\phi(\mathbf{r}) &= 1 - \frac{1}{4\pi^3}\int d^6r' \frac{1}{|\mathbf{r}-\mathbf{r}'|^4} V(\mathbf{r}')\phi(\mathbf{r}') \\ &= 1 + \hat{G}V\phi|_{\rho'>\rho_c} + \hat{G}V\phi|_{\rho'<\rho_c}\end{aligned}$$

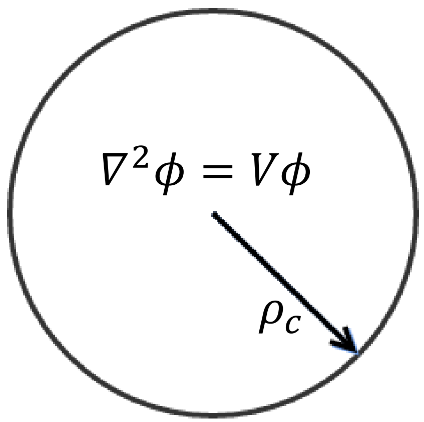
$\hat{G}V\phi|_{\rho'>\rho_c} = \sum_{nj} C_{nj}\rho^n\, Y_{nj}(\Omega)$ at $\rho \le \rho_c$, with KNOWN $C_{nj} = C_{nj}^{(0)} + C_{nj}^{(1)}D$

$\hat{G}V\phi|_{\rho'<\rho_c} = \sum_{nj} B_{nj}\rho^{-n-4}\, Y_{nj}(\Omega)$ at $\rho \ge \rho_c$, UNKNOWN

At $\rho = \rho_c$, $\phi = 1 + \sum_{nj}(C_{nj}\rho^n + B_{nj}\rho^{-n-4})Y_{nj}(\Omega)$, and its radial derivative

$$\frac{\partial\phi}{\partial\rho} = \sum_{nj}[nC_{nj}\rho^{n-1} - (n+4)B_{nj}\rho^{-n-5}]Y_{nj}(\Omega)$$

Matrix F



- For any Dirichlet boundary condition, ϕ at $\rho < \rho_c$ is completely determined. So,

$$\frac{\partial \phi}{\partial \rho}|_{\rho=\rho_c} = F(\rho_c)\phi|_{\rho=\rho_c}$$

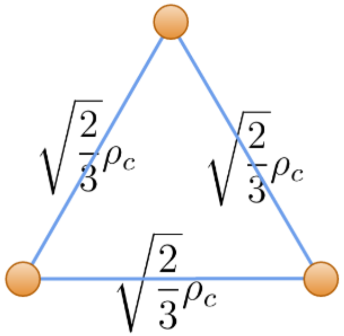
- F is a power series of ρ_c at small ρ_c, and

$$\frac{dF(\rho_c)}{d\rho_c} + F^2 + \frac{5}{\rho_c}F = \frac{\Lambda(\Omega)}{\rho_c^2} + \mathcal{V}(\rho_c)$$

- Found F at $\rho_c = 12$

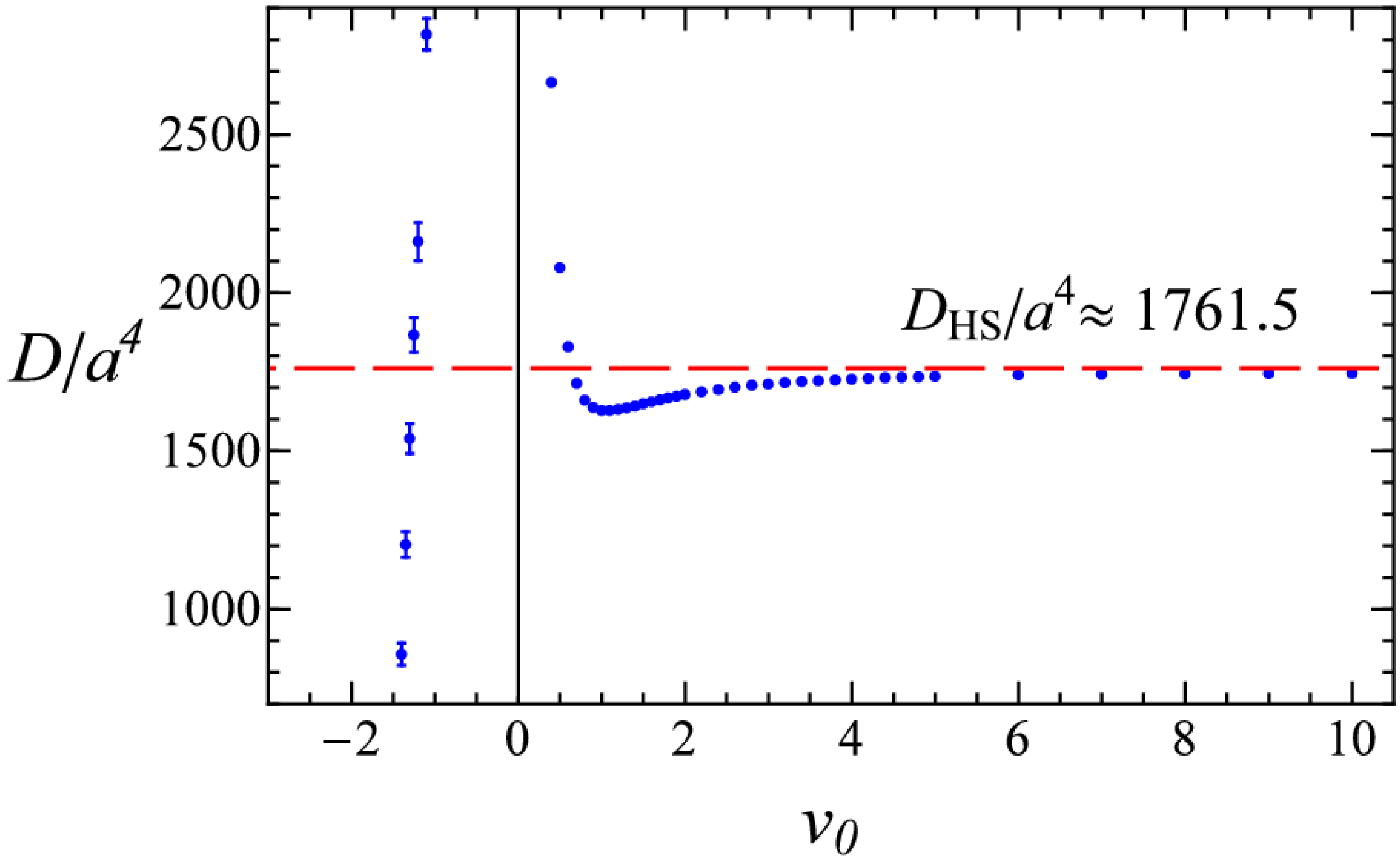
Determine D

- At $\rho = \rho_c$, $\phi = 1 + \sum_{nj}(C_{nj}\rho^{n} + B_{nj}\rho^{-n-4})Y_{nj}(\Omega)$, and
$$\frac{\partial\phi}{\partial\rho} = \sum_{nj}[nC_{nj}\rho^{n-1} - (n+4)B_{nj}\rho^{-n-5}]Y_{nj}(\Omega)$$
- From F and $C_{nj} = C_{nj}^{(0)} + C_{nj}^{(1)}D$, found $B_{nj} = B_{nj}^{(0)} + B_{nj}^{(1)}D$
- Then, compare

$\phi($ 

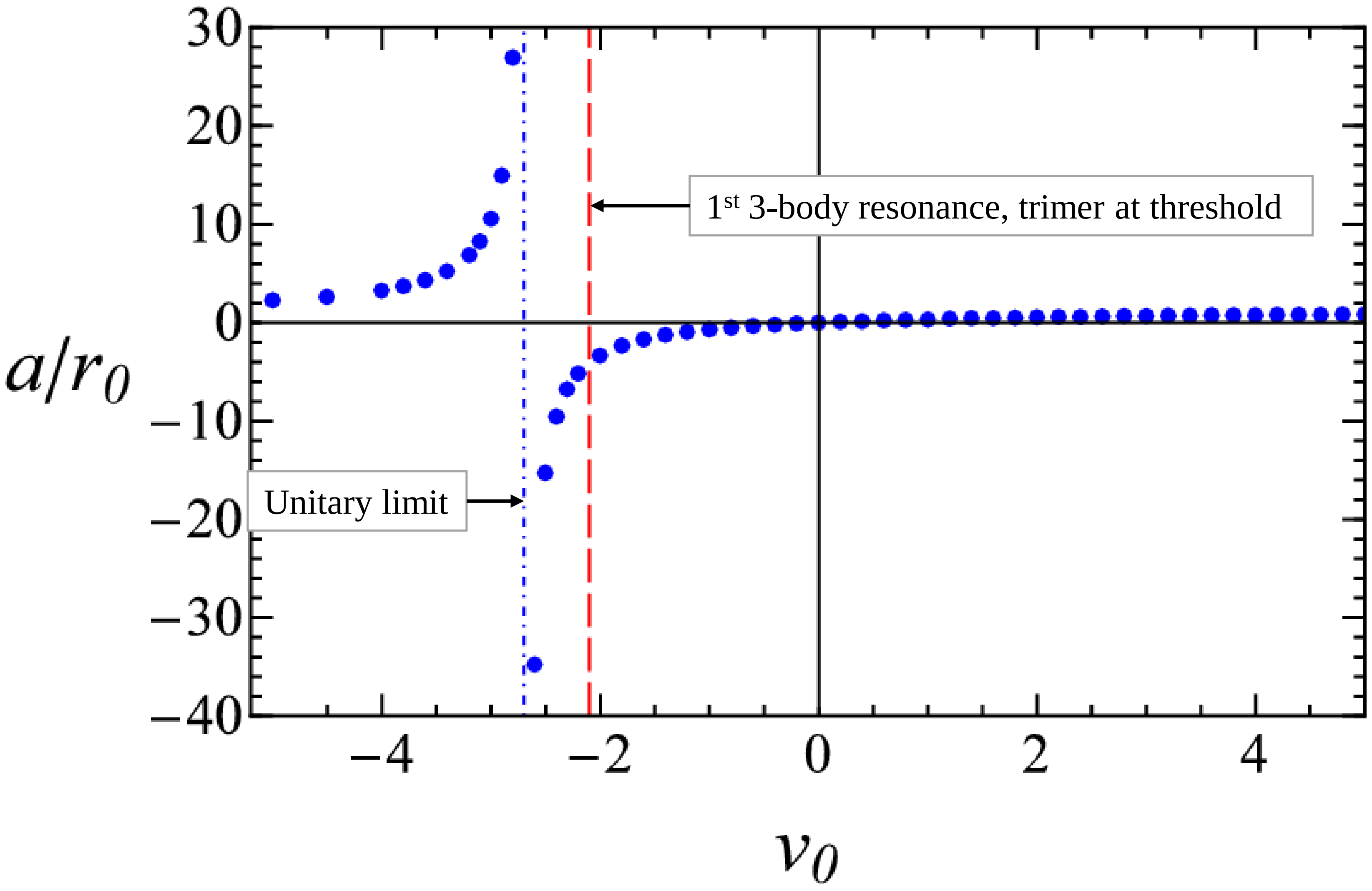
$)$ with the 111-expansion to determine D

D for soft-sphere boson



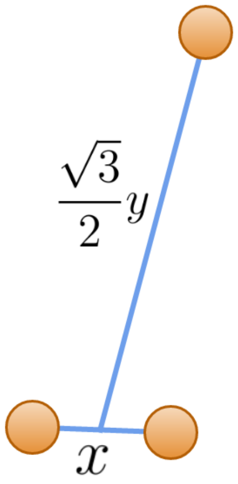
$$V(r) = \frac{v_0}{r_0^2} \exp(-r^2/r_0^2)$$

3-body resonance

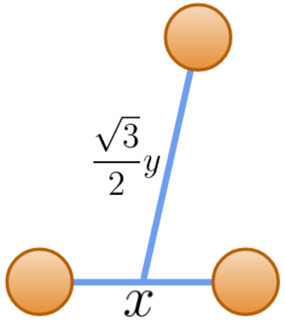


$$V(r) = \frac{v_0}{r_0^2}\exp(-r^2/r_0^2)$$

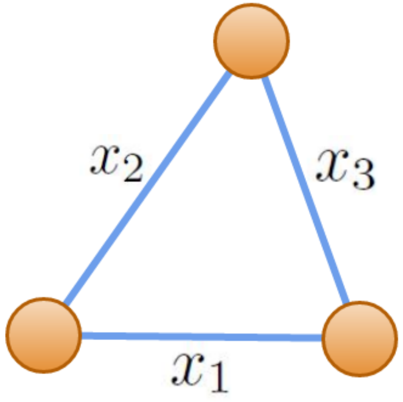
Extensions – unified formulas



$\cdots$



$\cdots$



- 21-expansion at $x \sim 1$
- Error $\sim \rho^{-8}$

- Intermediate region $x \sim \rho^{1/3}$
- Improved errors $\sim \rho^{-6} \to \sim \rho^{-8}$

- 111-expansion at $x_i \sim \rho$
- Error $\sim \rho^{-8}$

$$\rho = \frac{\sqrt{3}}{2}\sqrt{x^2 + y^2} = \sqrt{\frac{x_1^2 + x_2^2 + x_3^2}{2}}$$

Extensions

- With two-body bound states, $\mathrm{Im}D$ is related to the three-body recombination rate
- van der Waals tail $-1/r^6$, 21- and 111-expansions modified
- Two species (e.g. 1 light and 2 heavy atoms)
- Lower dimensions