Accuracy of the Born-Oppenheimer approximation and universality in a one-dimensional three-body system

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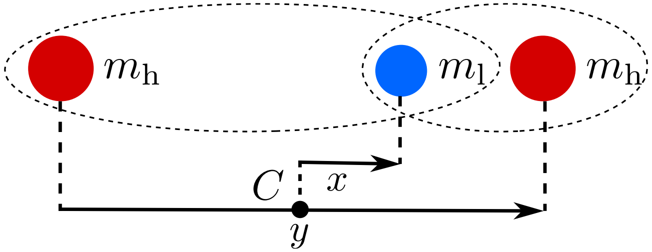
The system under consideration

- Two identical, heavy particles and one light particle
- One dimension
- No heavy-heavy interaction
- Contact heavy-light interaction
- Scaling in units of the two-body binding energy



Three-body Schrödinger equation

$$\left\{-\alpha_x \frac{\partial^2}{\partial x^2} - \alpha_y \frac{\partial^2}{\partial y^2} - 2\left[\delta(x+y/2) + \delta(x-y/2)\right]\right\}\psi(x,y) = \epsilon\,\psi(x,y)$$

$$\alpha_{x,y} = \alpha_{x,y}(m_\mathrm{h}/m_\mathrm{l})$$

Goals and Outline

- Accuracy of the Born-Oppenheimer approximation for three-body systems

→ Extend previous studies, e.g. Mehta, *PRA* **89**, 52706 (2014), Kartavtsev et al., *JETP* **108**, 365 (2009)

- Universality of three-body systems for short-range two-body interactions

→ Put universality on a more solid foundation

Born, Oppenheimer (BO): Adiabatic approximation

Separation ansatz; relying on large mass ratios

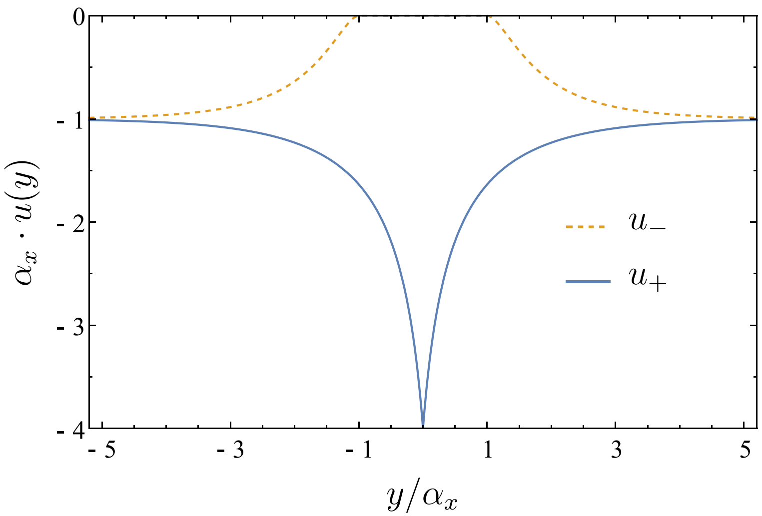
$$\psi_{\mathrm{BO}}(x,y) = \varphi(x|y)\chi(y)$$

Equation for the light particle

$$\left\{-\alpha_x \frac{\partial^2}{\partial x^2} - 2\left[\delta(x+y/2) + \delta(x-y/2)\right]\right\}\varphi = u(y)\varphi$$

Equation for the heavy particles

$$\left[-\alpha_y \frac{\partial^2}{\partial y^2} + u_+(y)\right]\chi = \epsilon^{(\mathrm{BO})}\chi$$



Skorniakov, Ter-Martirosian (STM): Exact Method

Solution of the Schrödinger equation in terms of the Green function

$$\psi(x,y) = -2\iint \mathrm{d}x'\mathrm{d}y' G_\epsilon(x-x', y-y')\psi(x',y')\left[\delta\left(x'+y'/2\right)+\delta\left(x'-y'/2\right)\right]$$

$$G_\epsilon(x,y) = -\frac{1}{2\pi\sqrt{\alpha_x\alpha_y}}K_0\left(\sqrt{|\epsilon|}\sqrt{\frac{1}{\alpha_x}x^2+\frac{1}{\alpha_y}y^2}\right)$$

Equation for the total wave function

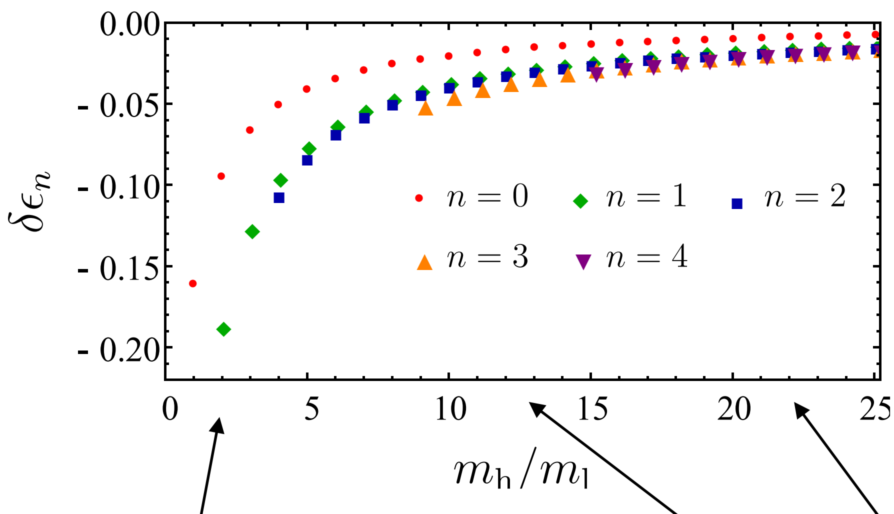
$$\psi(x,y) = -4\int \mathrm{d}x'\left[G_\epsilon(x-x', y-2x') \pm G_\epsilon(x-x', y+2x')\right]\psi(x',2x')$$

One-dimensional integral equation to obtain $\psi(x,2x)$ and ϵ

$$\sqrt{|\epsilon|}\,\psi(x,2x) = -4\int \mathrm{d}x'\left[G_1(x-x', 2x-2x') \pm G_1(x-x', 2x+2x')\right]\psi(x',2x')$$

Note: Equivalent equation can be derived using Bethe-Peierls boundary condition

BO vs. STM: Energy spectrum



$$\frac{m(^{87}\mathrm{Rb})}{m(^{40}\mathrm{K})} \simeq 2.2$$

$$\frac{m(^{87}\mathrm{Rb})}{m(^{7}\mathrm{Li})} \simeq 12.4$$

$$\frac{m(^{133}\mathrm{Cs})}{m(^{6}\mathrm{Li})} \simeq 22.2$$

Relative deviation

$$\delta\epsilon_n \equiv \frac{\epsilon_n^\star - \epsilon_n^{(\mathrm{BO})}}{\epsilon_n^\star}$$

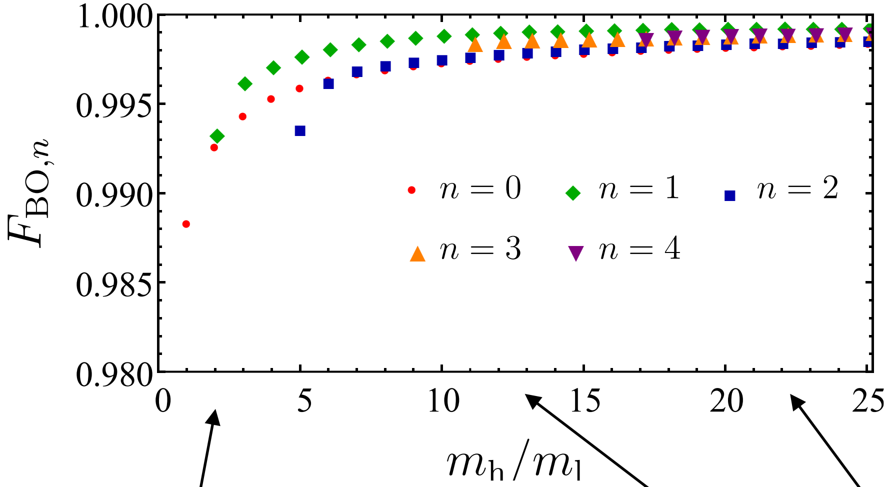
$\underline{m_\mathrm{h} = m_\mathrm{l}:}$

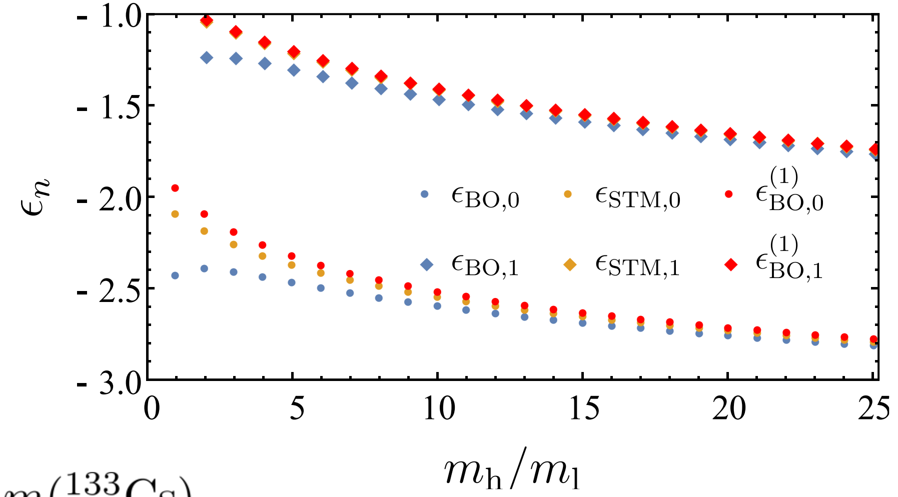
$\epsilon_0^{(\mathrm{BO})} = -2.42267$ (BO) $\qquad \epsilon_0^\star = -2.087719$ (STM)

Mehta, *PRA* **89**, 052706 (2014): -2.4227 (BO)

Kartavtsev et al., *JETP* **108**, 365 (2009): -2.087719 (HRE)

BO vs. STM: Wave function





$$\frac{m(^{133}\mathrm{Cs})}{m(^{6}\mathrm{Li})} \simeq 22.2$$

$$\frac{m(^{87}\mathrm{Rb})}{m(^{7}\mathrm{Li})} \simeq 12.4$$

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Fidelity

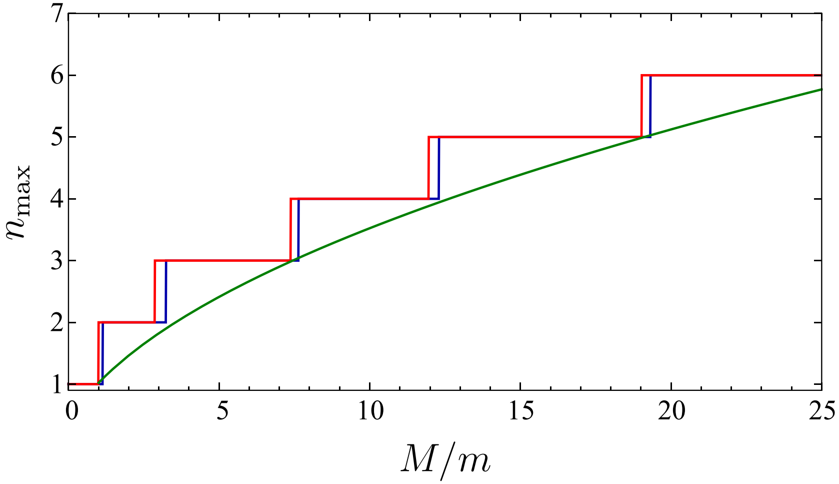
$$F_{\mathrm{BO},n} \equiv \langle \psi_n^{(\mathrm{BO})} | \psi_n^\star \rangle^2$$

Diagonal correction

$$\epsilon_n^{(\mathrm{BO},1)} \equiv \langle \psi_{\mathrm{BO},n} | \hat{H} | \psi_{\mathrm{BO},n} \rangle$$

BO vs. STM: Number of bound states

Numerical results (BO, STM)



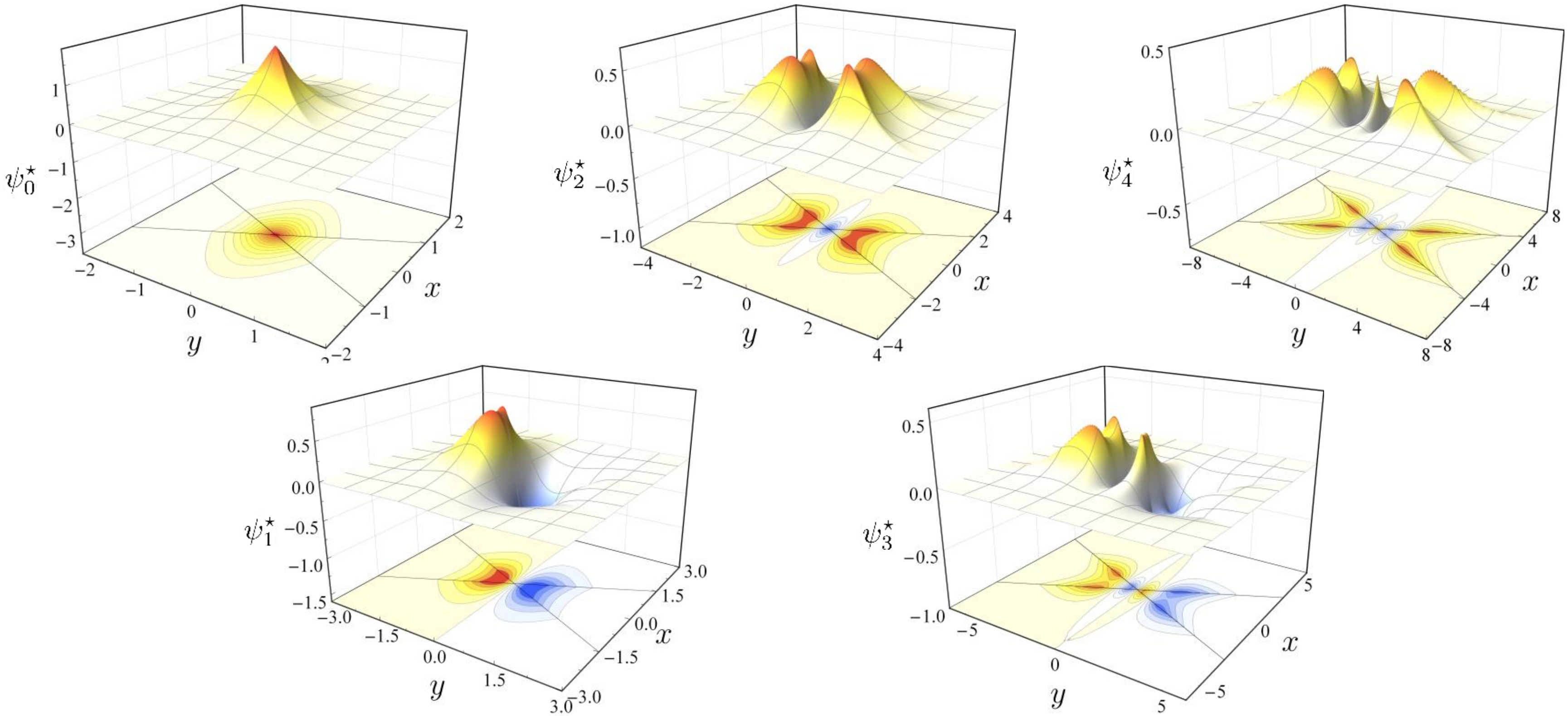
Semiclassical estimation

$$n_{\max} \simeq \frac{1}{\pi\sqrt{\alpha_y}} \int \mathrm{d}y \sqrt{|u_+(y) + 1/\alpha_y|} - \frac{1}{2}$$

$$n_{\max} \simeq 0.8781 \times \sqrt{1 + 2m_{\mathrm{h}}/m_{\mathrm{l}}} - 1/2$$

BO allows for a good and analytical estimation of the number of three-body bound states

Three-body wave functions (STM)



Lines of interaction $y = \pm 2x$

$$\frac{m_{\mathrm{h}}}{m_{\mathrm{l}}} = 20$$

y-symmetry: bosons (even), fermions (odd)
x-symmetry: always even

Universality

Energy of a weakly bound two-body ground state

$$\mathcal{E}_g^{(2)} \simeq \frac{1}{2}\left[\int \mathrm{d}x\, v_0 f(x)\right]^2$$

Three-body energies (contact interaction)

$$\epsilon_n^\star = \epsilon_n^\star(m_\mathrm{h}/m_\mathrm{l})$$

Independent of v_0

	atomic mixture (M/m)		
	^{87}Rb–^{40}K (2.2)	^{87}Rb–^{7}Li (12.4)	^{133}Cs–^{6}Li (22.2)
$\epsilon_0^\star$	-2.1966	-2.5963	-2.7515
$\epsilon_1^\star$	-1.0520	-1.4818	-1.6904
$\epsilon_2^\star$	-	-1.1970	-1.3604
$\epsilon_3^\star$	-	-1.0377	-1.1479
$\epsilon_4^\star$	-	-1.0002	-1.0525
$\epsilon_5^\star$	-	-	-1.0040

How universal are these „constants“?

Universality

Two finite-range potentials

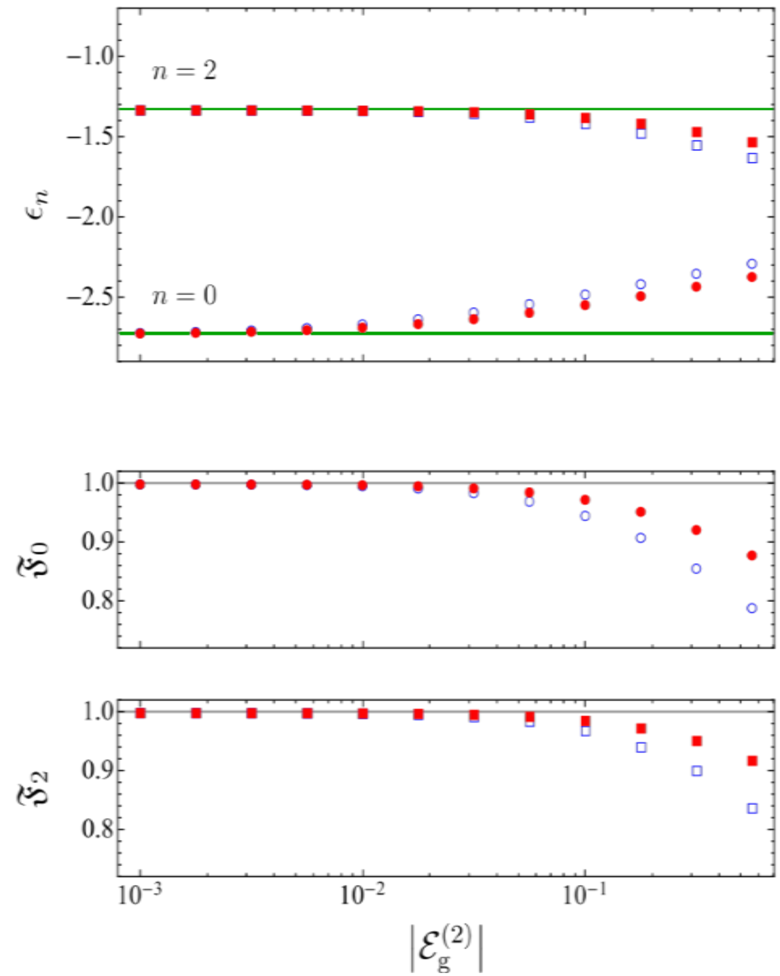
$$v_{\mathrm{G}}(x) = v_0 \mathrm{e}^{-x^2} \qquad v_{\mathrm{L}}(x) = v_0 \frac{1}{(1+x^2)^3}$$

Universal three-body energies

$$\mathcal{E}_n^{(3)} \simeq \frac{1}{2}\epsilon_n^\star \left[\int \mathrm{d}x \, v_0 f(x) \right]^2$$

$$v_\delta(x) = v_0 \delta(x)$$

Proof for **any** short-range potential (including wave functions)



Only valid close to the two-body ground-state resonance!

Conclusion and Outlook

- Accuracy of the BO approximation for three-body systems:
  - Deviation in the energy spectrum drops from around 20% to below 2% with increasing mass ratio
  - Wave functions are closely matched with fidelities up to 0.999
  - Diagonal correction further reduces energy deviation
  - Analytical estimation of the number trimers

- Universality:
  - Proof of universal three-body behavior in energies and wave functions close to the two-body ground-state resonance

L. Happ, et al. *PRA* **100**, 012709 (2019)

- Outlook:
  - Analyze universality for other two-body resonances

Collaboration

Thank you for your attention.