Two and Three-Body Systems with Synthetic Spin-Orbit Coupling

Qingze Guan

1.Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklahoma

2.Center for Quantum Research and Technology, The University of Oklahoma, Norman, Oklahoma

3. Department of Physics and Astronomy, Washington State University, Pullman, Washington

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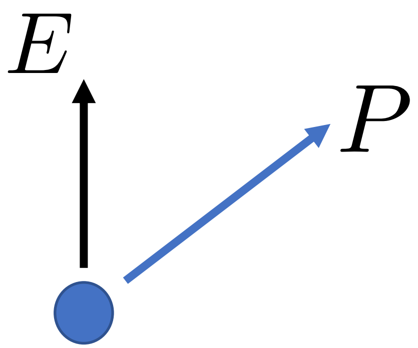
Spin-Orbit Coupling (Spin-Momentum Coupling)

- In atomic physics, we have seen the spin orbit coupling due to relativistic correction. The SOC term has the form of $\mathbf{L} \cdot \mathbf{S}$.

- In condensed matter physics, a different type of SOC (spin-momentum coupling) also exists, e.g., the $\mathbf{P} \times \mathbf{S}$ and $\mathbf{P} \cdot \mathbf{S}$ terms.

- A native picture for one type of SOC:



A charged particle moving in E-field!

- Effective B-field due to relativistic correction:

$$B = -\frac{p \times E}{mc}$$

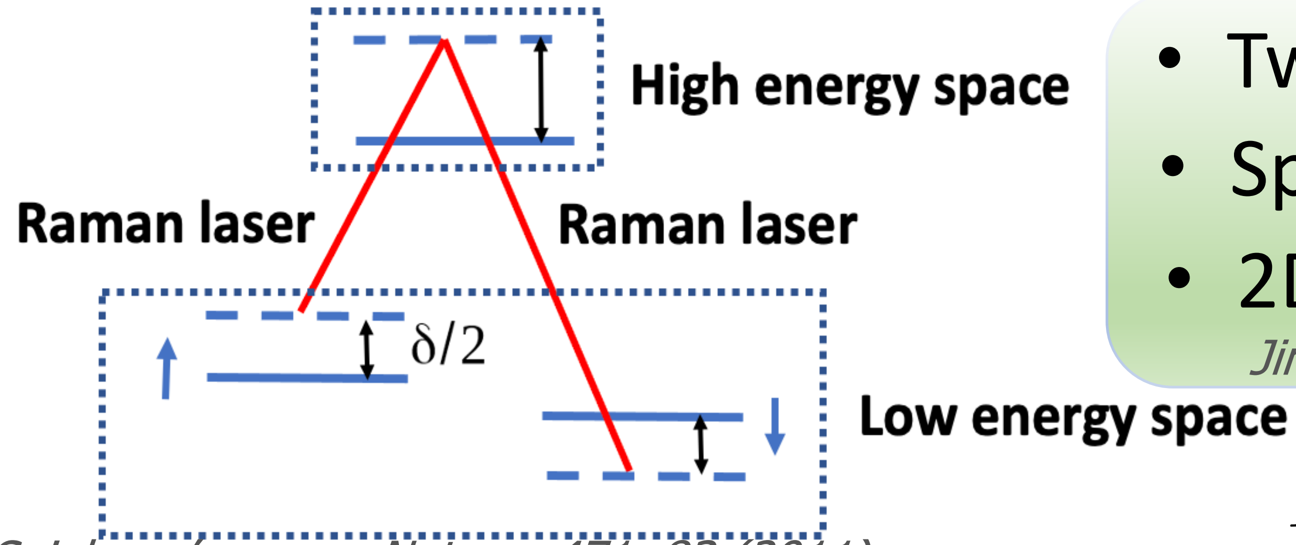
- B-field interacts with spin:

$$H_{so} = \alpha(\mathbf{p} \times \mathbf{S}) \cdot E$$

Synthetic 1D SOC

- There are many types of SOC: Rashba SOC, Dresselhaus SOC, mixture of Rashba and Dresselhaus SOC, Weyl SOC, …

- The SOC terms can be synthetically realized using neutral cold atoms, e.g., the NIST Raman laser scheme for equal mixture of Rashba and Dresselhaus SOC (or 1D SOC),



Spielman's group, Nature 471, 83 (2011).

- Two-photon process
- Spin-flip locked to momentum kick
- 2D isotropic SOC also realized

Jing Zhang's group, Nat. Phys. 12, 540 (2016).

$$H^{soc} = \frac{\mathbf{p}^2}{2m} + \frac{\hbar k_{so}}{m} p_z \sigma_z + \frac{\Omega}{2}\sigma_x + \frac{\delta}{2}\sigma_z$$

3D Isotropic (Weyl) SOC---Single Particle

- Single-particle Hamiltonian: $$H_{1\mathrm{b}} = \frac{\mathbf{p}^2}{2m} + \frac{\hbar k_{so}}{m}\mathbf{p}\cdot\sigma \qquad \sigma = (\sigma_{\mathbf{x}}, \sigma_{\mathbf{y}}, \sigma_{\mathbf{z}})$$
- Two-branch dispersion relationship:

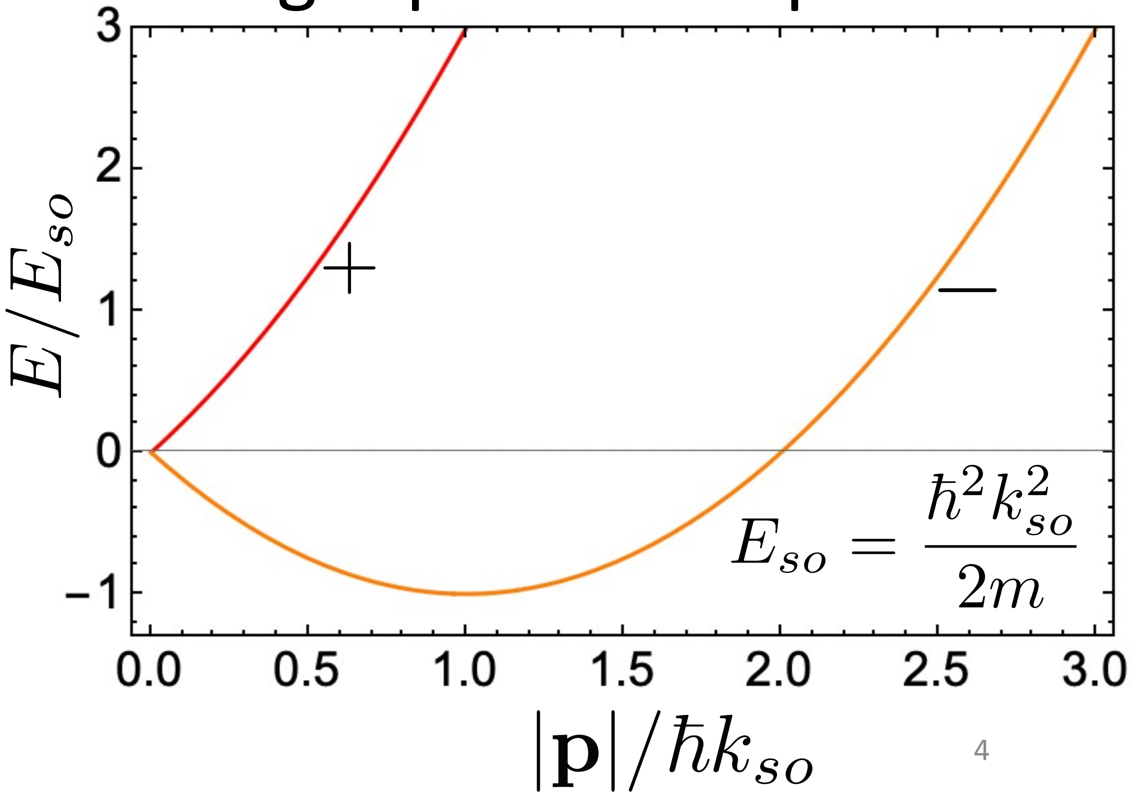
Positive helicity: $\xrightarrow{\sigma^+}$ $\longrightarrow \mathbf{p}$

$$E^+ = p^2/2m + \hbar k_{so} p/m$$

Negative helicity: $\xleftarrow{\sigma^-}$ $\longrightarrow \mathbf{p}$

$$E^- = p^2/2m - \hbar k_{so} p/m$$

Single-particle dispersion



3D Isotropic (Weyl) SOC---Two Particles

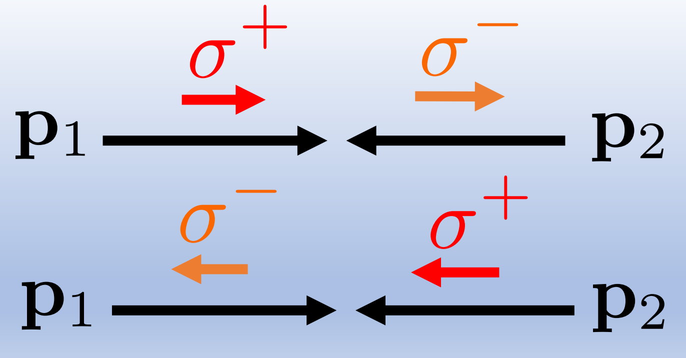
- Two-body NI Hamiltonian: $$H_{2b} = \left(\frac{\mathbf{p_1^2}}{2m} + \frac{\mathbf{p_2^2}}{2m}\right) + \frac{\hbar k_{so}}{m}\left(\mathbf{p_1}\cdot\sigma_\mathbf{1} + \mathbf{p_2}\cdot\sigma_\mathbf{2}\right)$$

- In the COM frame: $\mathbf{P} = \mathbf{p_1} + \mathbf{p_2} = \mathbf{0}$

$$H_{\rm rel} = \frac{\mathbf{p}_{\rm rel}^\mathbf{2}}{2\mu} + \frac{\hbar k_{so}}{\mu}\mathbf{p}_{\rm rel}\cdot\left(\frac{\sigma_\mathbf{1} - \sigma_\mathbf{2}}{\mathbf{2}}\right)$$

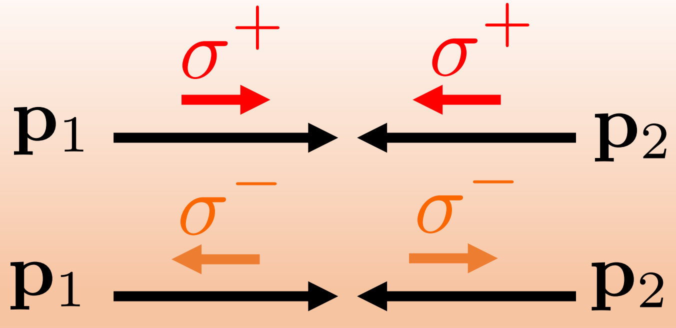
(+,-) helicity:

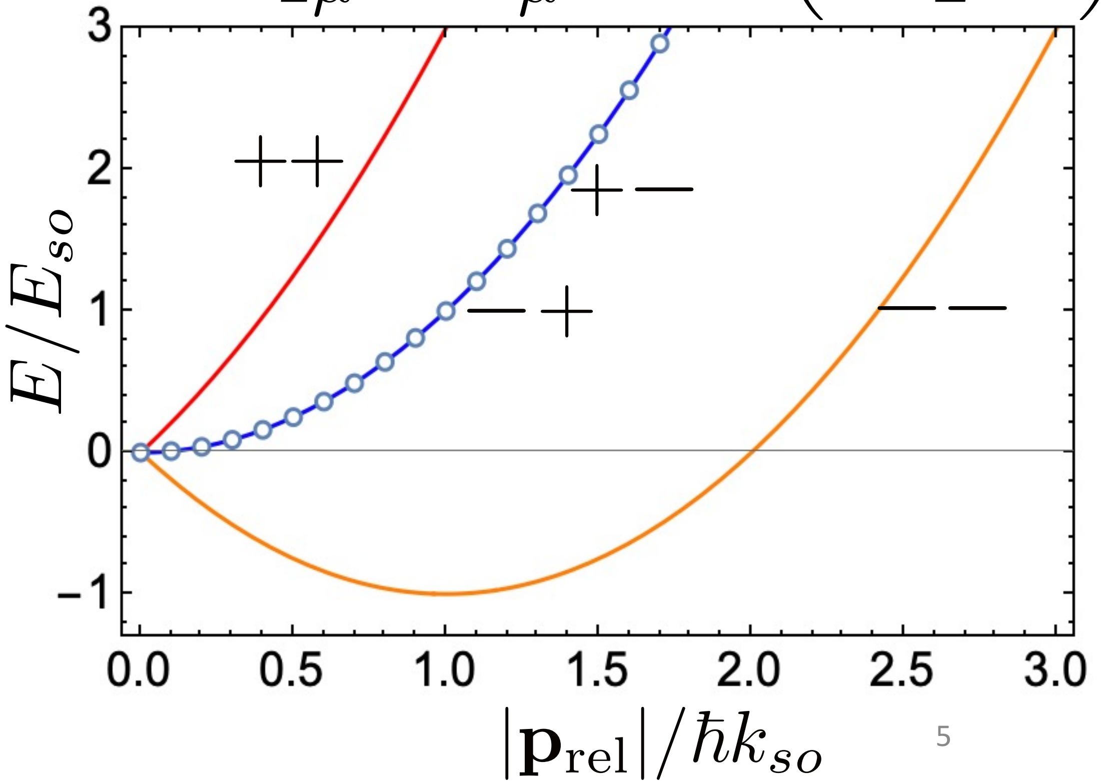
(-,+) helicity:



(+,+) helicity:

(-,-) helicity:





3D Isotropic (Weyl) SOC---Total Angular Momentum Conservation

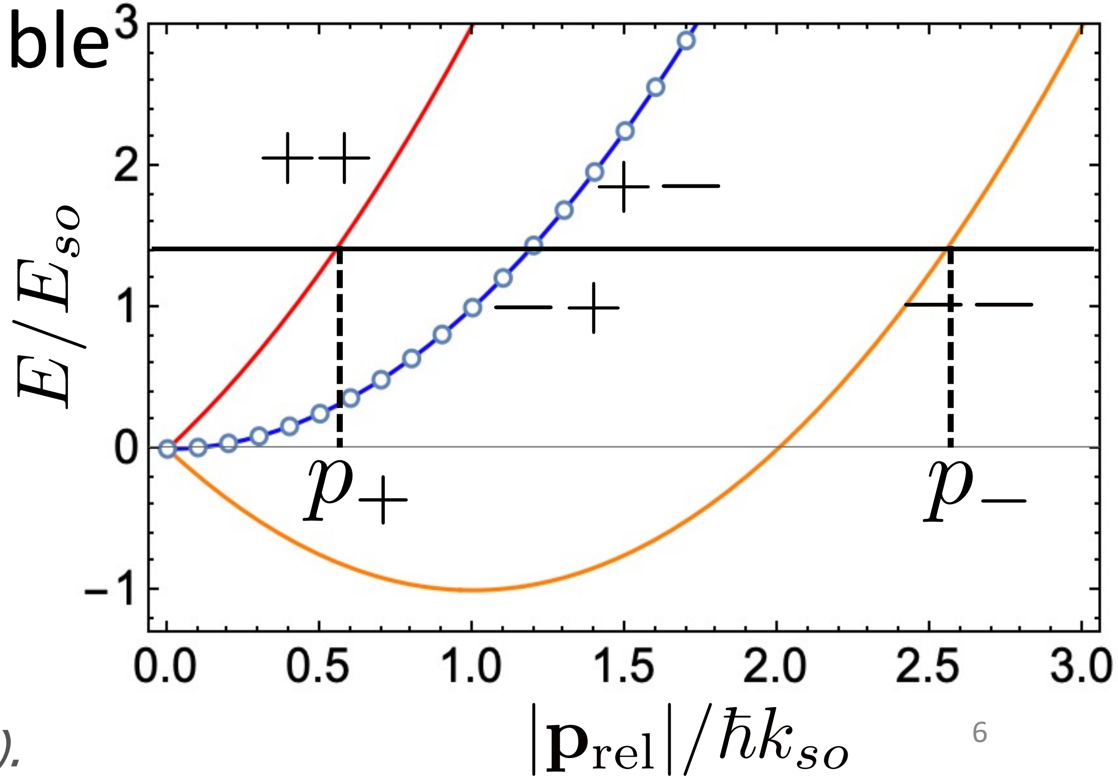
- Two-body interacting Hamiltonian:

$$H_{\rm rel} = \frac{\mathbf{p}_{\rm rel}^2}{2\mu} + \frac{\hbar k_{so}}{\mu}\mathbf{p}_{\rm rel}\cdot\left(\frac{\sigma_1-\sigma_2}{2}\right) + V_{\rm 2b}(|\mathbf{r}_{\rm rel}|)$$

The total angular momentum J=L+S is conserved!

- Focus on the J=0 channel, two possible angular momentum combinations:

$$|J=0, M=0; L=0, S=0\rangle$$
$$|J=0, M=0; L=1, S=1\rangle$$



- Only the “++” and “--” branches matter for the J=0 channel.

See also H. Duan, L. You, and B. Gao, PRA 87, 052708 (2013).

3D Isotropic (Weyl) SOC---2Body Scattering Solution

- For a short-range potential, the asymptotic scattering solution:

$$\psi(r) \xrightarrow{r\to\infty} \mathcal{J}(r) - \mathcal{N}(r)\mathcal{K}$$

K-matrix includes the scattering phase shift

- Regular solution (E>0):

$$\begin{array}{cccc} & ++ & -- & \\ \mathcal{J}(r) = & \left[\begin{array}{c} \frac{\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} j_0\left(\frac{p_+ r}{\hbar}\right) \\ \frac{-i\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} j_1\left(\frac{p_+ r}{\hbar}\right) \end{array}\right. & \left.\begin{array}{c} \frac{\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} j_0\left(\frac{p_- r}{\hbar}\right) \\ \frac{-i\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} j_1\left(\frac{p_- r}{\hbar}\right) \end{array}\right] & \begin{array}{c} |J=0, M=0; L=0, S=0\rangle \\ |J=0, M=0; L=1, S=1\rangle \end{array} \end{array}$$

- Irregular solution (E>0):

$$\begin{array}{cccc} \mathcal{N}(r) = & \left[\begin{array}{c} \frac{\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} n_0\left(\frac{p_+ r}{\hbar}\right) \\ \frac{-i\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} n_1\left(\frac{p_+ r}{\hbar}\right) \end{array}\right. & \left.\begin{array}{c} \frac{\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} n_0\left(\frac{p_- r}{\hbar}\right) \\ \frac{-i\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} n_1\left(\frac{p_- r}{\hbar}\right) \end{array}\right] & \begin{array}{c} |J=0, M=0; L=0, S=0\rangle \\ |J=0, M=0; L=1, S=1\rangle \end{array} \end{array}$$

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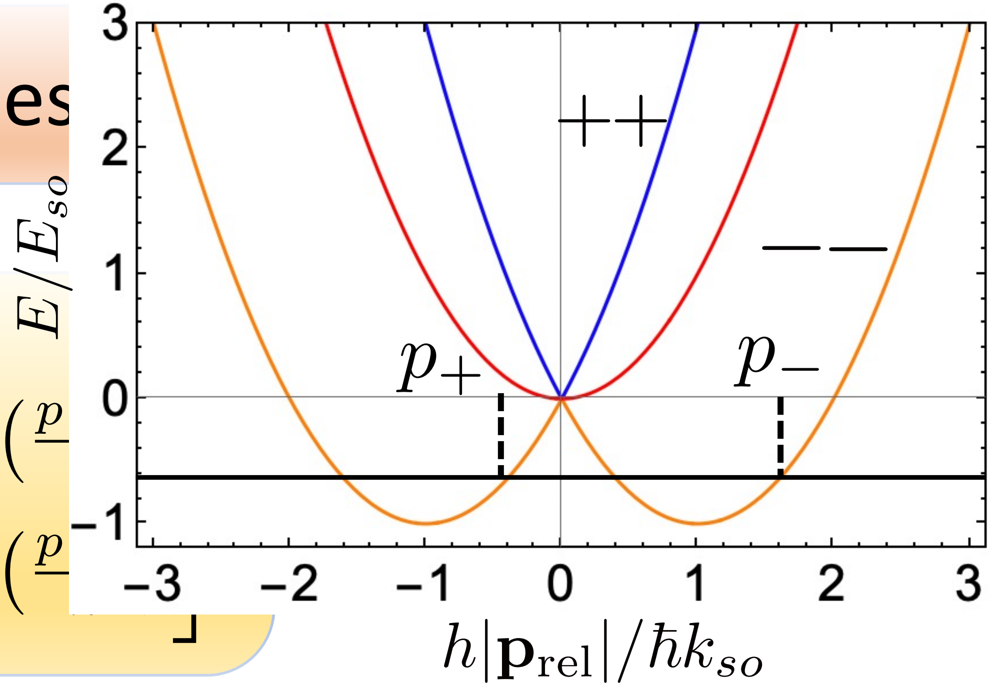
K-matrix includes



- Regular solution (E<0):

$$\begin{array}{ccc} & -- & -- \\ \mathcal{J}(r) = & \left[\begin{matrix} \frac{\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} j_0\left(\frac{p_+ r}{\hbar}\right) & \frac{\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} j_0\left(\frac{p}{}\cdots\right) \\ \frac{-i\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} j_1\left(\frac{p_+ r}{\hbar}\right) & \frac{-i\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} j_1\left(\frac{p}{}\cdots\right) \end{matrix}\right] \end{array}$$

- Irregular solution (E<0):

$$\mathcal{N}(r) = \left[\begin{matrix} \frac{\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} n_0\left(\frac{p_+ r}{\hbar}\right) & \frac{\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} n_0\left(\frac{p_- r}{\hbar}\right) \\ \frac{-i\sqrt{\mu}p_+}{\sqrt{2(p_+ + k_{so})}} n_1\left(\frac{p_+ r}{\hbar}\right) & \frac{-i\sqrt{\mu}p_-}{\sqrt{2(p_- - k_{so})}} n_1\left(\frac{p_- r}{\hbar}\right) \end{matrix}\right]$$

Helicity:

$$h = \frac{\left\langle \mathbf{p}_{\rm rel} \cdot \frac{\sigma_1 - \sigma_2}{2} \right\rangle}{\left|\left\langle \mathbf{p}_{\rm rel} \cdot \frac{\sigma_1 - \sigma_2}{2} \right\rangle\right|}$$

3D Isotropic (Weyl) SOC---2Body Scattering Solution

- For zero-range s-wave interaction and vanishing p-wave interaction:

K-matrix: $$\mathcal{K} = -\frac{a_s}{k_+ - k_-}\begin{bmatrix} k_+^2 & k_+k_- \\ k_+k_- & k_-^2 \end{bmatrix} \qquad k_\pm = \pm\sqrt{2\mu(E+E_{so})} - \hbar k_{so}$$

- Eigenvalues of K-matrix: $$\tan\delta^s_{\text{eff}} = -a_s k_{\text{so}}\left[\underbrace{\left(\frac{E}{E_{\text{so}}}+1\right)^{1/2}}_{\text{3D DOS}} + \underbrace{\left(\frac{E}{E_{so}}+1\right)^{-1/2}}_{\text{1D DOS}}\right]$$

Effective dimension reduction: 3D DOS 1D DOS

The other eigenvalue is zero since no p-wave phase shift is included!

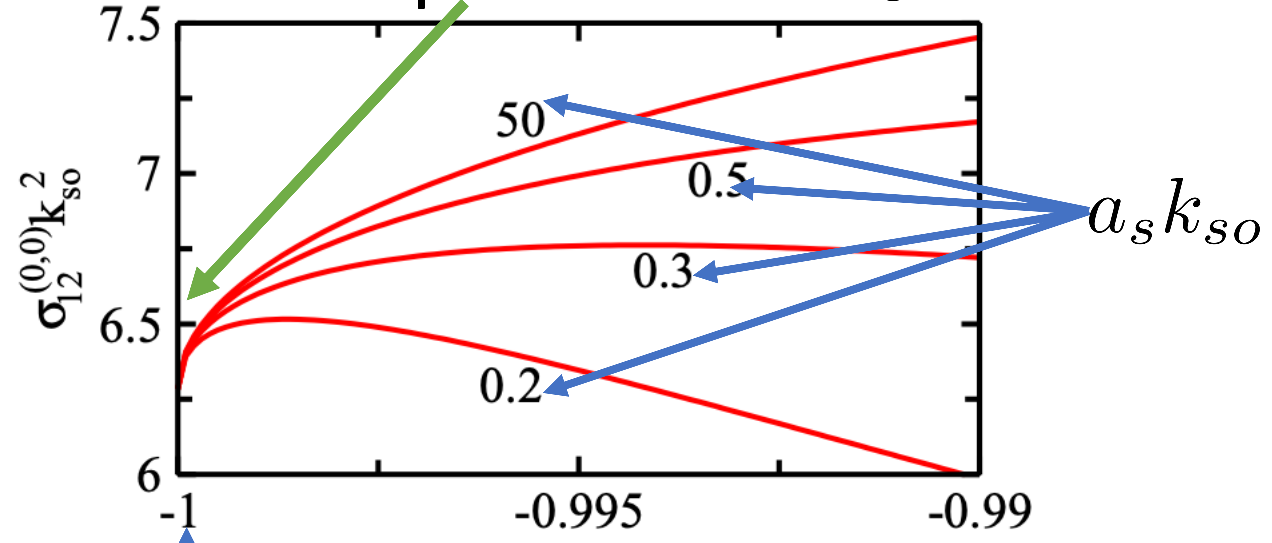
3D Isotropic (Weyl) SOC---Effects of Dimension Reduction

- Scattering cross sections:

S-matrix: $\mathcal{S} = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}$

Cross-section: $\sigma_{jl} = \dfrac{2\pi\hbar^2}{p_j^2} \left|\mathcal{S}_{jl} - \delta_{jl}\right|^2$

independent of a_s

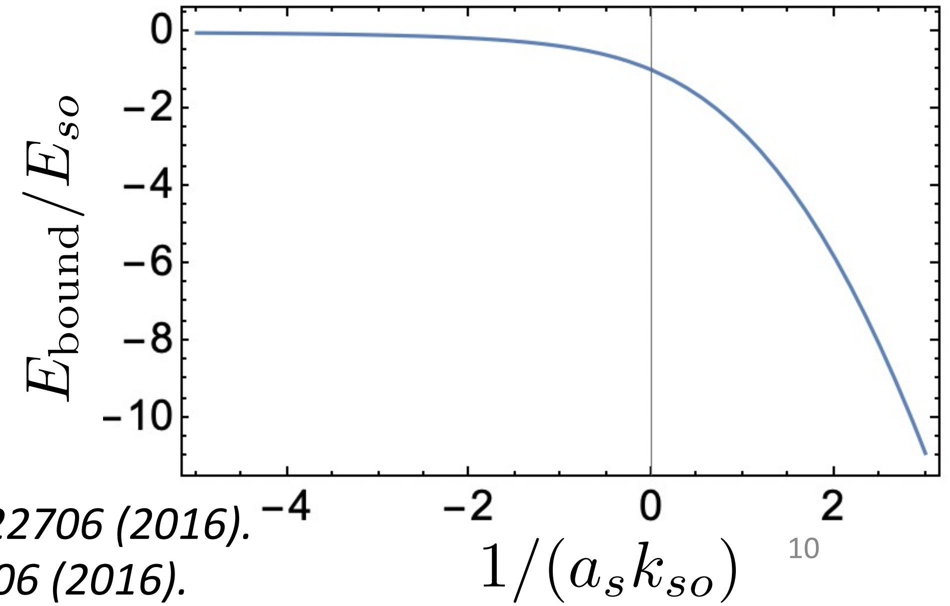


- Enhanced binding:

$\tan \delta^s_{\text{eff}} = -i \qquad E_{\text{binding}} = -\dfrac{\hbar^2 k_*^2}{2\mu}$

$$k^* = \frac{1 + \mathrm{sgn}(a_s)\sqrt{1 + 4a_s^2 k_{so}^2}}{2a_s}$$

bound state exists for negative a_s



*[1] S.-J. Wang and C. Greene, PRA **91**, 022706 (2016).*
*[2]Q. Guan and D. Blume, PRA **94**, 022706 (2016).*

3D Isotropic (Weyl) SOC---Short-Range Boundary Condition?

- I have not told you what boundary condition I used to obtain the analytical K matrix.

- Question: how do the SOC terms interplay with the short-range phase shift?

- The results are for vanishing p-wave interaction. Since SOC couples s- and p-wave, how to include the p-wave phase-shift?.

- The question we asked: given the scattering length and scattering volume for the system without SOC, how to obtain the solution for the SOC system?

3D Isotropic (Weyl) SOC---Rotated Hamiltonian

- Two-body interacting Hamiltonian:

$$H_{\rm rel} = \underbrace{\frac{\mathbf{p}_{\rm rel}^2}{2\mu}}_{O\left(r_{\rm rel}^{-2}\right)} + \underbrace{\frac{\hbar k_{so}}{\mu}\mathbf{p}_{\rm rel}\cdot\left(\frac{\sigma_1-\sigma_2}{2}\right)}_{O\left(r_{\rm rel}^{-1}\right)} + V_{\rm 2b}(|\mathbf{r}_{\rm rel}|)$$

We count $p_{\rm rel} \sim O\left(r_{\rm rel}^{-1}\right)$

Define a rotation operator

$$R = e^{\frac{-ik_{so}(\sigma_1-\sigma_2)\cdot\mathbf{r}_{\rm rel}}{2}}$$

- Rotated two-body Hamiltonian:

$$R^{-1}H_{\rm rel}R = \underbrace{\frac{\mathbf{p}_{\rm rel}^2}{2\mu} + V_{\rm 2b}(|\mathbf{r}_{\rm rel}|)}_{\text{No SOC Hamiltonian}} + \underbrace{iE_{\rm so}\left[\frac{(\sigma_1-\sigma_2)\cdot\mathbf{r}_{\rm rel}}{2}, \frac{(\sigma_1-\sigma_2)\cdot\mathbf{p}_{\rm rel}}{2}\right]}_{O(1)} + \underbrace{O(r_{\rm rel})}_{\text{Neglected}}$$

3D Isotropic (Weyl) SOC--- Effective Channel-Dependent Scattering Energy

- For the J=0 channel, the matrix form of the O(1) order term:

$$iE_{\mathrm{so}}\left[\frac{(\sigma_1-\sigma_2)\cdot\mathbf{r}_{\mathrm{rel}}}{2},\frac{(\sigma_1-\sigma_2)\cdot\mathbf{p}_{\mathrm{rel}}}{2}\right]\to\begin{bmatrix}-3E_{so} & 0\\ 0 & E_{so}\end{bmatrix}$$

- In the short-distance region, the rotated s- and p-wave channels are similar to the non-SOC system, but at different scattering energies:

$$\left[\frac{\mathbf{p}_{\mathrm{rel}}^2}{2\mu}+V_{2\mathrm{b}}(|\mathbf{r}_{\mathrm{rel}}|)\right]\psi_s=(E+3E_{so})\psi_s \quad \left[\frac{\mathbf{p}_{\mathrm{rel}}^2}{2\mu}+V_{2\mathrm{b}}(|\mathbf{r}_{\mathrm{rel}}|)\right]\psi_p=(E-E_{so})\psi_p$$

- Given the full energy dependence of $a_s(E)$ and $V_p(E)$ including the negative energy regime, we can fully solve the SOC system.

3D Isotropic (Weyl) SOC--- The General Framework

- Evaluate the propagation of the different partial wave channel in short-distance region at these channel dependent scattering energy.

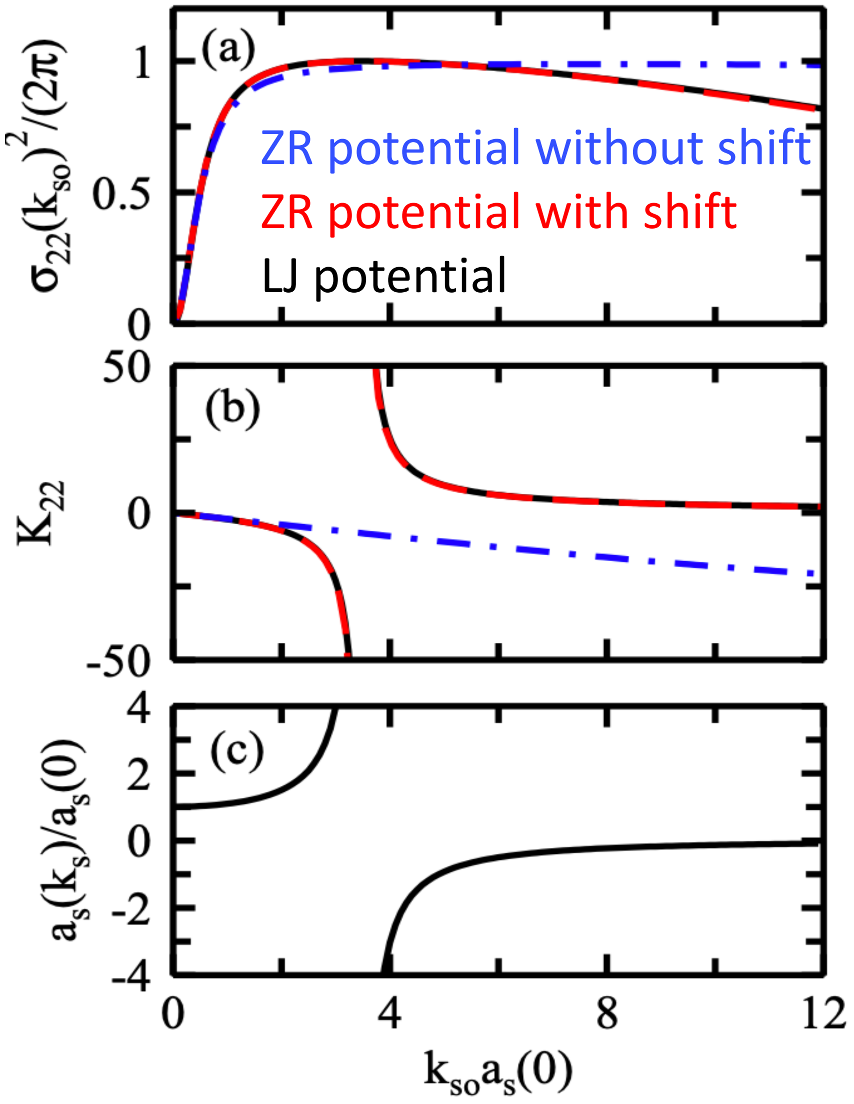
- Up to a large enough distance, i.e., the matching point, rotate the propagated scattering solution.

- Match the log derivative of the rotated inner solution to that of the asymptotic solution.

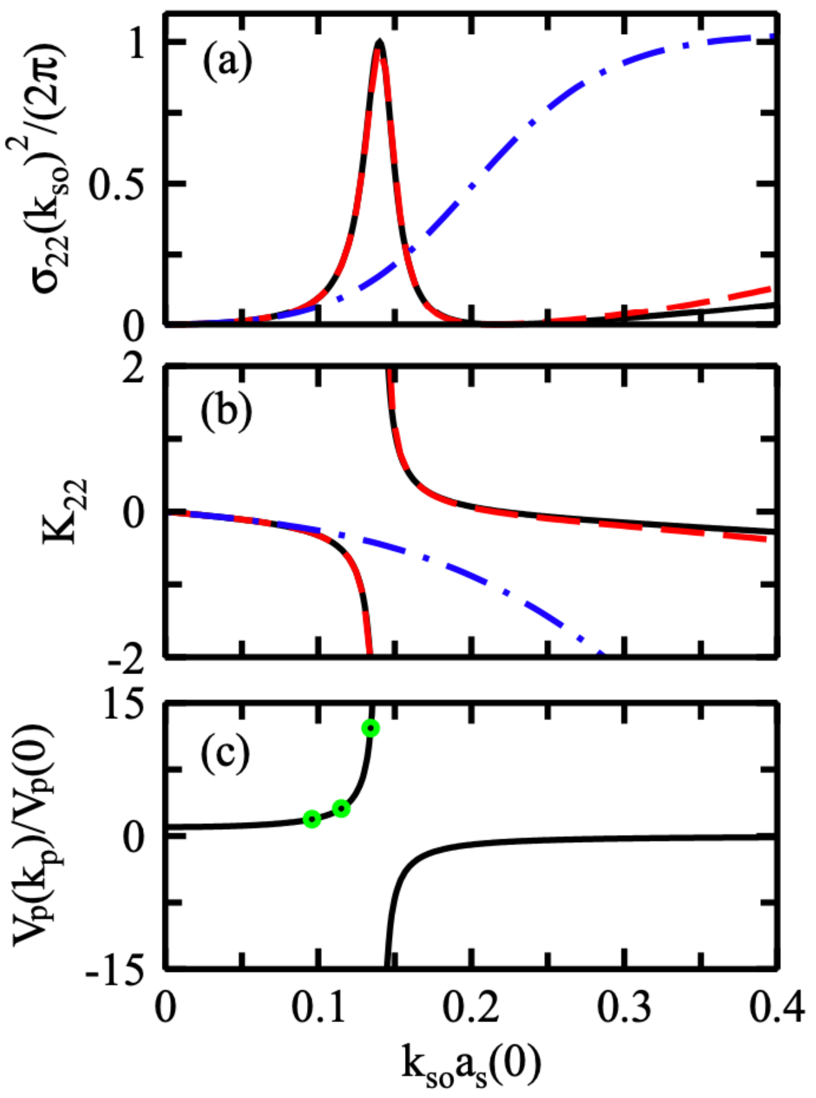
- For a zero-range pseudopotential, we can just match the rotated asymptotic solution to the normal boundary condition with a “renormalized” scattering phase shift.

3D Isotropic (Weyl) SOC--- Benchmark Analytical Solution

- Large a_s regime:



- Large V_p regime:



$$\hat{V}_{2b}(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$$

For large V_p, the energy shifts in the ZR model are crucial to describe the partial cross section.

Q. Guan and D. Blume, PRA ***95****, 020702(R) (2017).*

3D Isotropic (Weyl) SOC--- Breaking Galilean Invariance

- All the results are for vanishing COM momentum.
- For the SOC system, the value of the COM momentum enters the relative system Hamiltonian as an effective detuning, the so-called "breaking of Galilean invariance".

$$H_{\mathrm{rel}} = \frac{\mathbf{p}_{\mathrm{rel}}^2}{2\mu} + \frac{\hbar k_{so}}{\mu}\mathbf{p}_{\mathrm{rel}} \cdot \left(\frac{\sigma_1 - \sigma_2}{2}\right) + V_{2\mathrm{b}}(|\mathbf{r}_{\mathrm{rel}}|) + \frac{\hbar k_{so}}{M}\mathbf{P}_{\mathrm{com}} \cdot (\sigma_1 + \sigma_2)$$

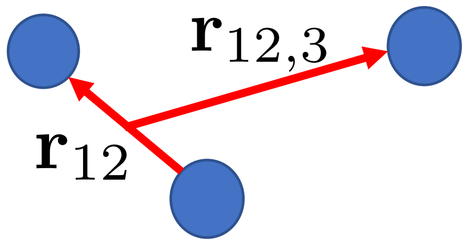
- A fixed finite COM momentum breaks the conservation of the total angular momentum and couples more partial waves together. Richer scattering solutions are expected. Future work!

3D Isotropic (Weyl) SOC--- Summary

- The dispersion relationship of the SOC system is different from the non-SOC system.
- The helicity can be used to understand the dispersion relationship in our head.
- The connection between the SOC system and the non-SOC system at short-distance is established.
- A general framework for the SOC scattering is discussed and analytical solutions are obtained in the P=0 space.
- The 3D SOC leads to an effective dimension reduction near the threshold, universal scattering cross section, enhanced binding,…

Three-Boson System without SOC

- Hamiltonian for 3 pairwise interacting bosons in COM frame:



$$H_{nosoc} = \frac{\hat{\mathbf{p}}_{12}^2}{2\mu_{12}} + \frac{\hat{\mathbf{p}}_{12,3}^2}{2\mu_{12,3}} + \Sigma_{i<j} V_{zr}(\mathbf{r}_{ij})$$

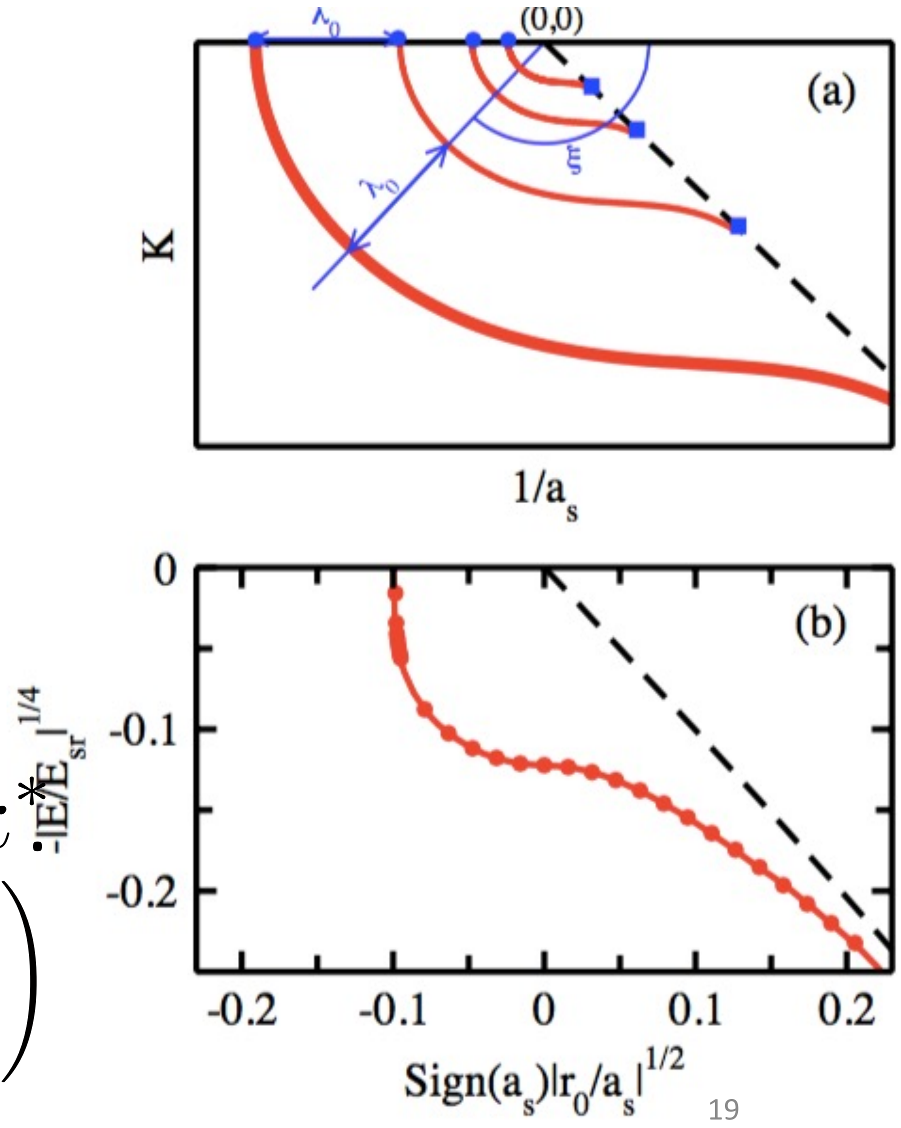
- The parameter space: $(a_s, K = -\sqrt{|E|m/\hbar^2}; \kappa^*)$

- Continuous scale invarianance: given a solution of SE for $(a_s, K; \kappa^*)$, a rescaled solution for $(a_s/\lambda, \lambda K; \lambda\kappa^*)$ also exists.

This is just saying we can always choose a unit of a physical system and make the equation dimensionless.

Three-Boson System without SOC---Radial Scaling Law

- Discrete radial scaling law: given a solution of SE for $(a_s, K; \kappa^*)$, a rescaled solution for $(a_s/\lambda_0, \lambda_0 K; \kappa^*)$ also exists. κ^* is not rescaled.
- Explicitly Correlated Gaussian approach (ECG): two-body Gaussian potential + three-body Gaussian potential. Dots: rescaled energy for rescaled a_s and fixed κ^*.



$$V_{2b}(r_{jk}) = v_0 \exp\left(-\frac{r_{jk}^2}{2r_0^2}\right) \quad V_{3b}(r_{jkl}) = V_0 \exp\left(-\frac{r_{jkl}^2}{2R_0^2}\right)$$

$$r_{jkl}^2 = r_{jk}^2 + r_{jl}^2 + r_{kl}^2$$

Three-Boson System with 1D SOC---Hamiltonian

- Single-particle Hamiltonian: $H^{soc} = \frac{\hat{\mathbf{p}}^2}{2m} \otimes I_2 + \frac{\hbar k_{so} p_z}{m}\sigma_z + \frac{\Omega}{2}\sigma_x + \frac{\delta}{2}\sigma_z$

- 3 particle Hamiltonian:

$$H = H_1^{SOC} + H_2^{SOC} + H_3^{SOC} + V_{2b}(r_{12}) + V_{2b}(r_{13}) + V_{2b}(r_{23}) + V_{3b}(R)$$

- Separating the COM and the relative d.o.f:

$$H = \frac{\mathbf{p}_{12}^2}{2\mu_{12}} + \frac{\mathbf{p}_{12,3}^2}{2\mu_{12,3}} + \frac{\hbar k_{so}}{m}\left[p_{12,z}(\sigma_{z,1} - \sigma_{z,2}) + p_{12,3,z}\left(\frac{\sigma_{z,1} + \sigma_{z,2}}{2} - \sigma_{z,3}\right)\right]$$
$$+ \frac{\Omega}{2}(\sigma_{x,1} + \sigma_{x,2} + \sigma_{x,3}) + \left(\frac{\delta}{2} + \frac{\hbar k_{so} P_{\mathrm{com},z}}{M}\right)(\sigma_{z,1} + \sigma_{z,2} + \sigma_{z,3})$$
$$+ V_{2b}(r_{12}) + V_{2b}(r_{13}) + V_{2b}(r_{23}) + V_{3b}(R) + \frac{\mathbf{P}_{\mathrm{COM}}^2}{2M}$$

$$\tilde{\delta} = \delta + \frac{2\hbar k_{so} P_{\mathrm{com},z}}{M}$$

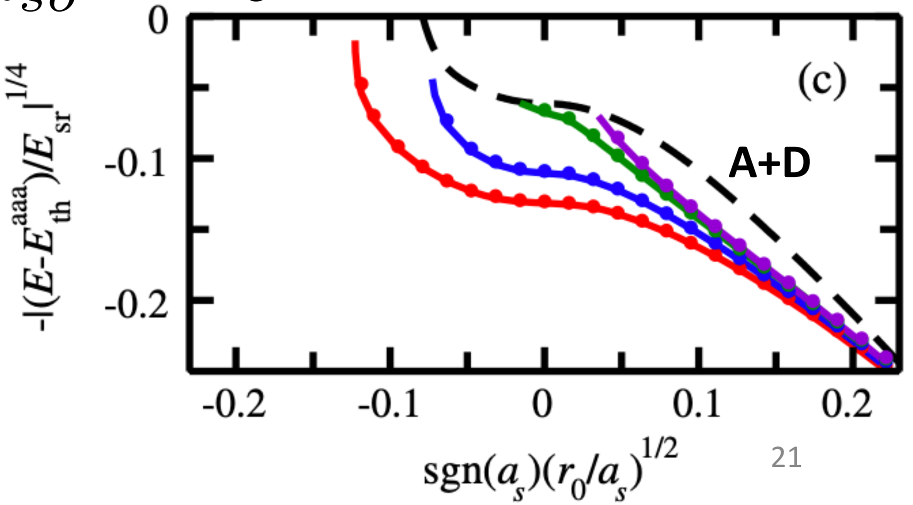
Three-Boson System with 1D SOC---Radial Scaling Law

- For three pseudospin-1/2 particle, there are 4 fully symmetric spin configuration: 3 $|\uparrow\rangle$, 2$|\uparrow\rangle$+1$|\downarrow\rangle$, 2$|\downarrow\rangle$+ 1$|\uparrow\rangle$, 3$|\downarrow\rangle$.
- Each 3-body curve gets spit into four curves due to the SOC terms.
- The parameter space for the 3body system: $(a_s, k_{so}, \tilde{\delta}, \Omega, K; \kappa^*)$
- A generalized radial scaling law:

$$\frac{1}{a_s} \rightarrow \frac{\lambda_0}{a_s}, k_{so} \rightarrow \lambda_0 k_{so}, \tilde{\delta} \rightarrow \lambda_0^2 \tilde{\delta},$$

$$\Omega \rightarrow \lambda_0^2 \Omega, K \rightarrow \lambda_0 K, \kappa^* \rightarrow \kappa^*$$

$\kappa^*/k_{so} \approx 1.5$



[1] Z.Y. Shi, X. Cui, and H. Zhai, PRL 112, 013201 (2014)
[2] Z.Y. Shi, H. Zhai, and X. Cui, PRA 91, 023618 (2015)
[3] Q. Guan and D. Blume, PRX 8, 021057 (2018)

Three-Boson System with 1D SOC---Scattering Threshold

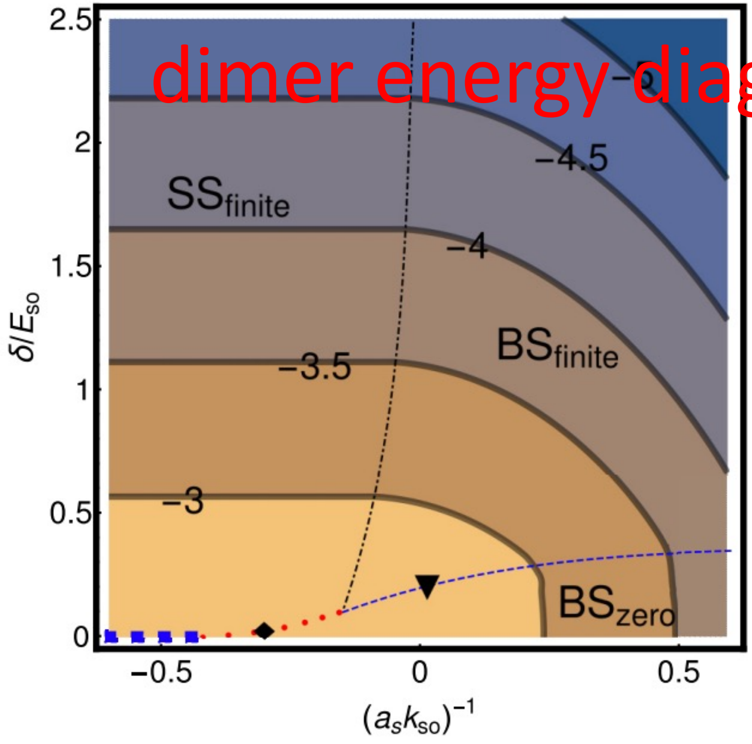
- 3Body scattering threshold: $\bar{E}_{3,\mathrm{rel,th}}(\tilde{\delta}) = \min\left[\bar{E}^{\mathrm{aaa}}_{3,\mathrm{rel,th}}(\tilde{\delta}), \bar{E}^{\mathrm{ad}}_{3,\mathrm{rel,th}}(\tilde{\delta})\right].$

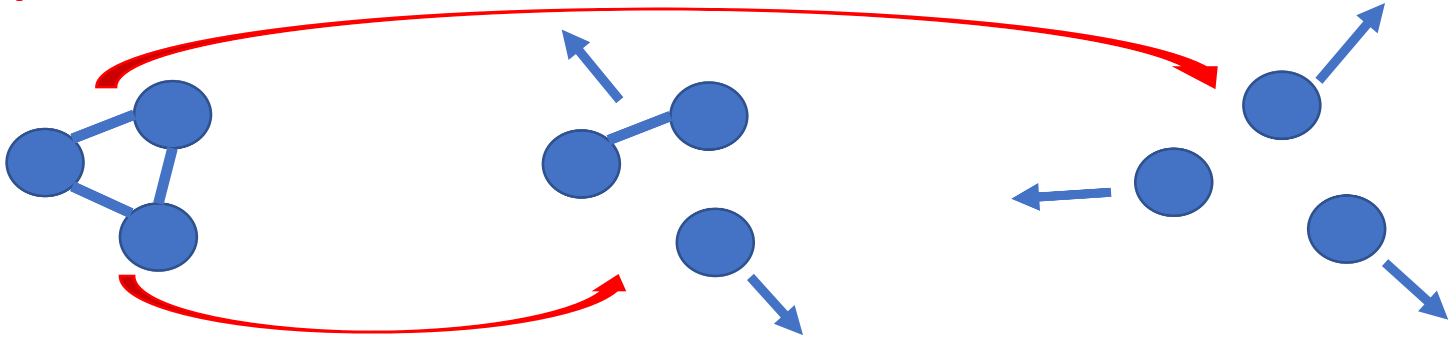
3 Atom threshold:

$$\bar{E}^{\mathrm{aaa}}_{3,\mathrm{rel,th}}(\tilde{\delta}) = \min_{\vec{q}_1,\vec{q}_2}\left[\bar{E}^{(0)}_{3,\mathrm{rel,ni}}(\vec{q}_1, \vec{q}_2, \tilde{\delta})\right]$$

Atom+Dimer threshold:

$$\bar{E}^{\mathrm{ad}}_{3,\mathrm{rel,th}}(\tilde{\delta}) = \min_{\vec{q}_2}\left[\bar{E}^{(0)}_{2,\mathrm{rel}}\left(\tilde{\delta} + \frac{\hbar k_{\mathrm{so}} q_{2,z}}{m}\right) + \bar{E}^{(0)}_{2,\mathrm{rel,ni}}\left(\vec{q}_2, \tilde{\delta} - \frac{2\hbar k_{\mathrm{so}} q_{2,z}}{m}\right) - \frac{\vec{q}_2^{\,2}}{4m}\right]$$



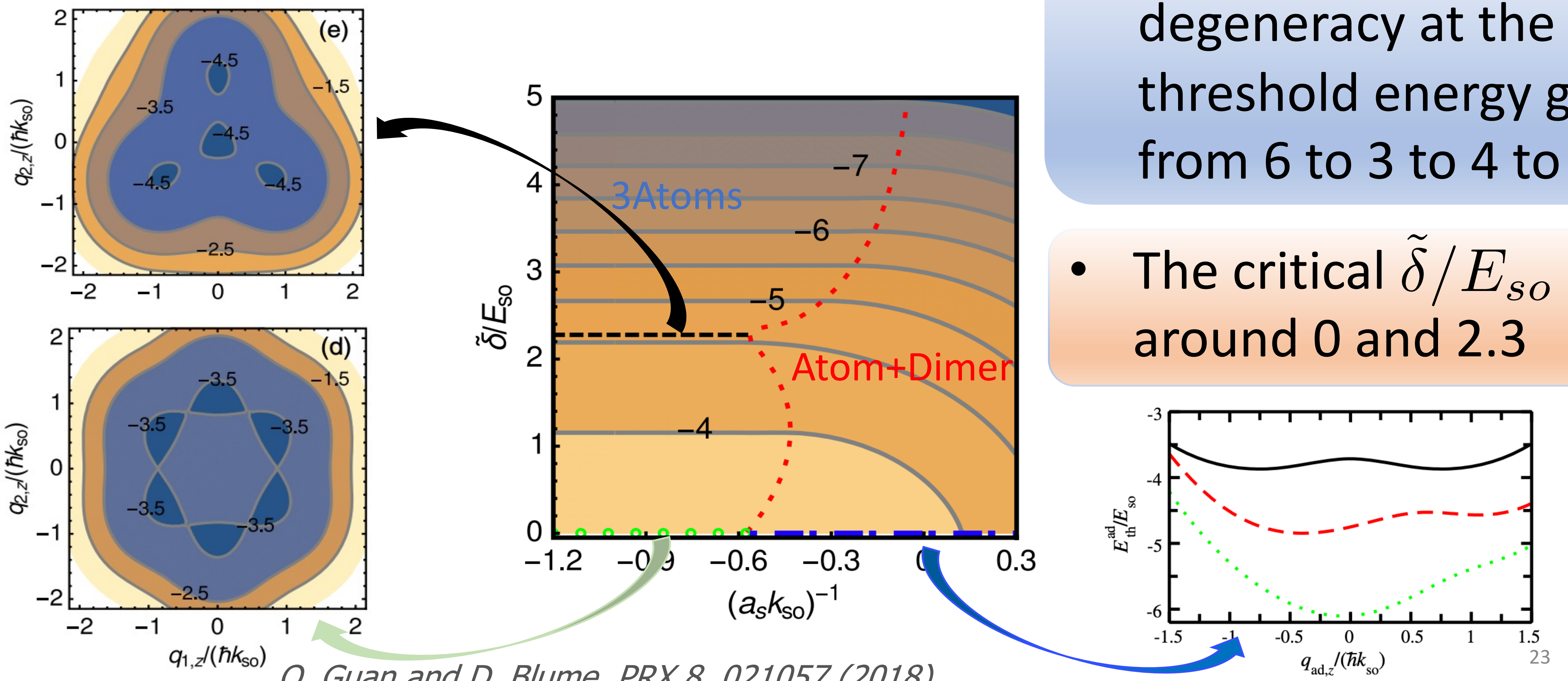


To determine 3-body threshold, the full COM dependence of the dimer energy is needed!

Q. Guan and D. Blume, PRA 100, 042708 (2019)

Three-Boson System with 1D SOC---Scattering Threshold

- 3Body scattering threshold:



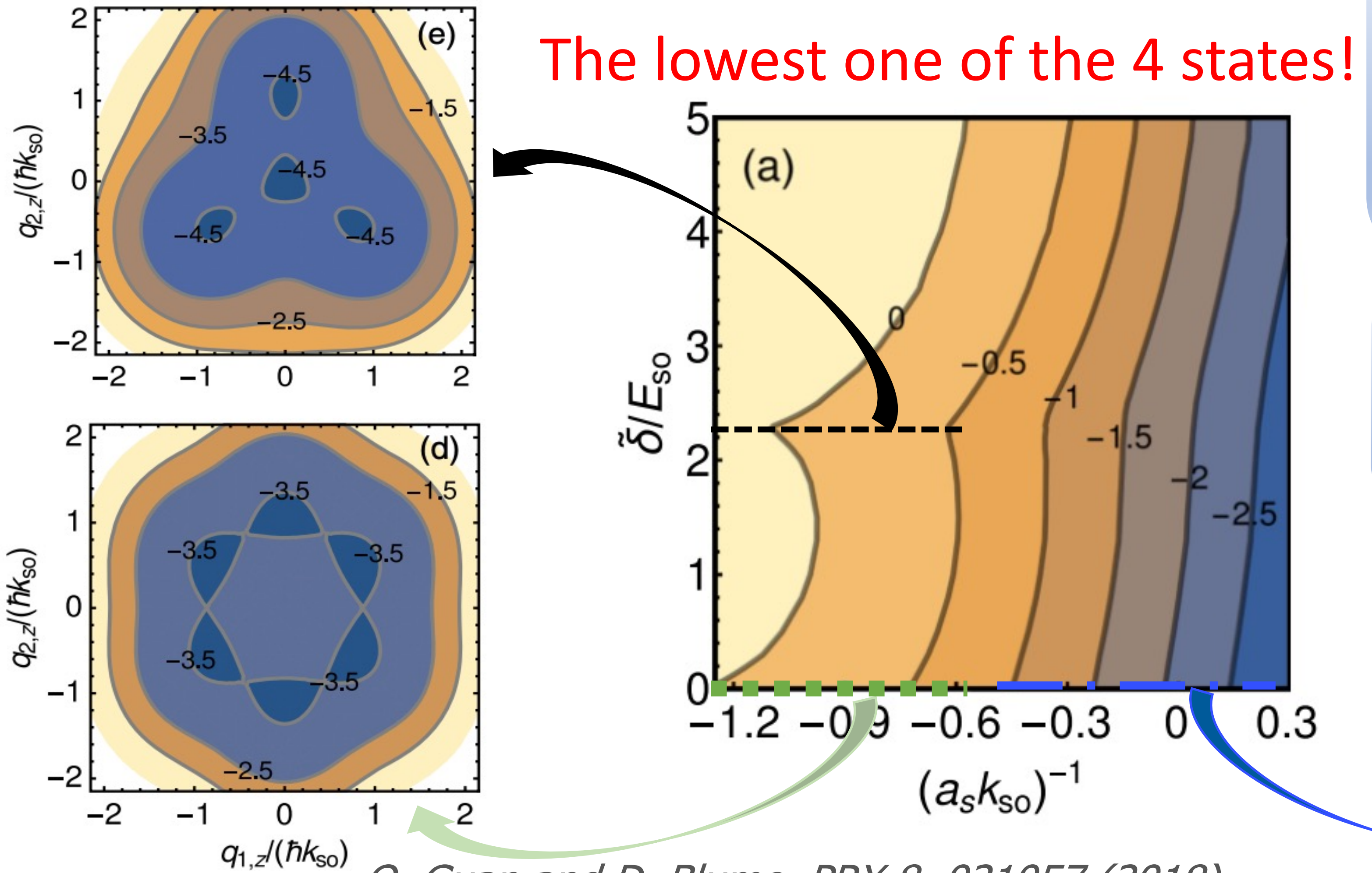
- The number of degeneracy at the threshold energy goes from 6 to 3 to 4 to 1!

- The critical $\tilde{\delta}/E_{so}$ are around 0 and 2.3

Q. Guan and D. Blume, PRX 8, 021057 (2018)

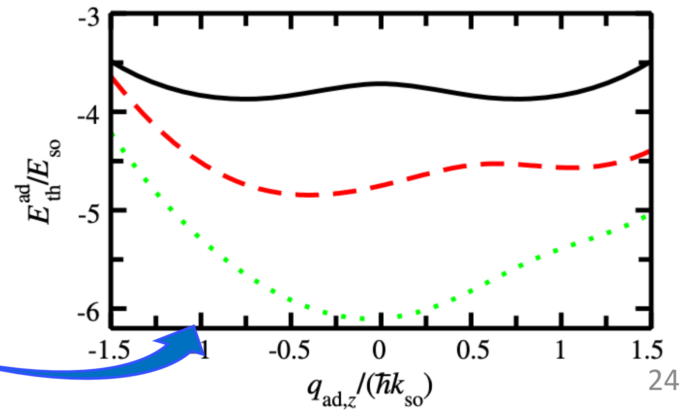
Three-Boson System with 1D SOC---Binding Energy

- 3Body binding energy:



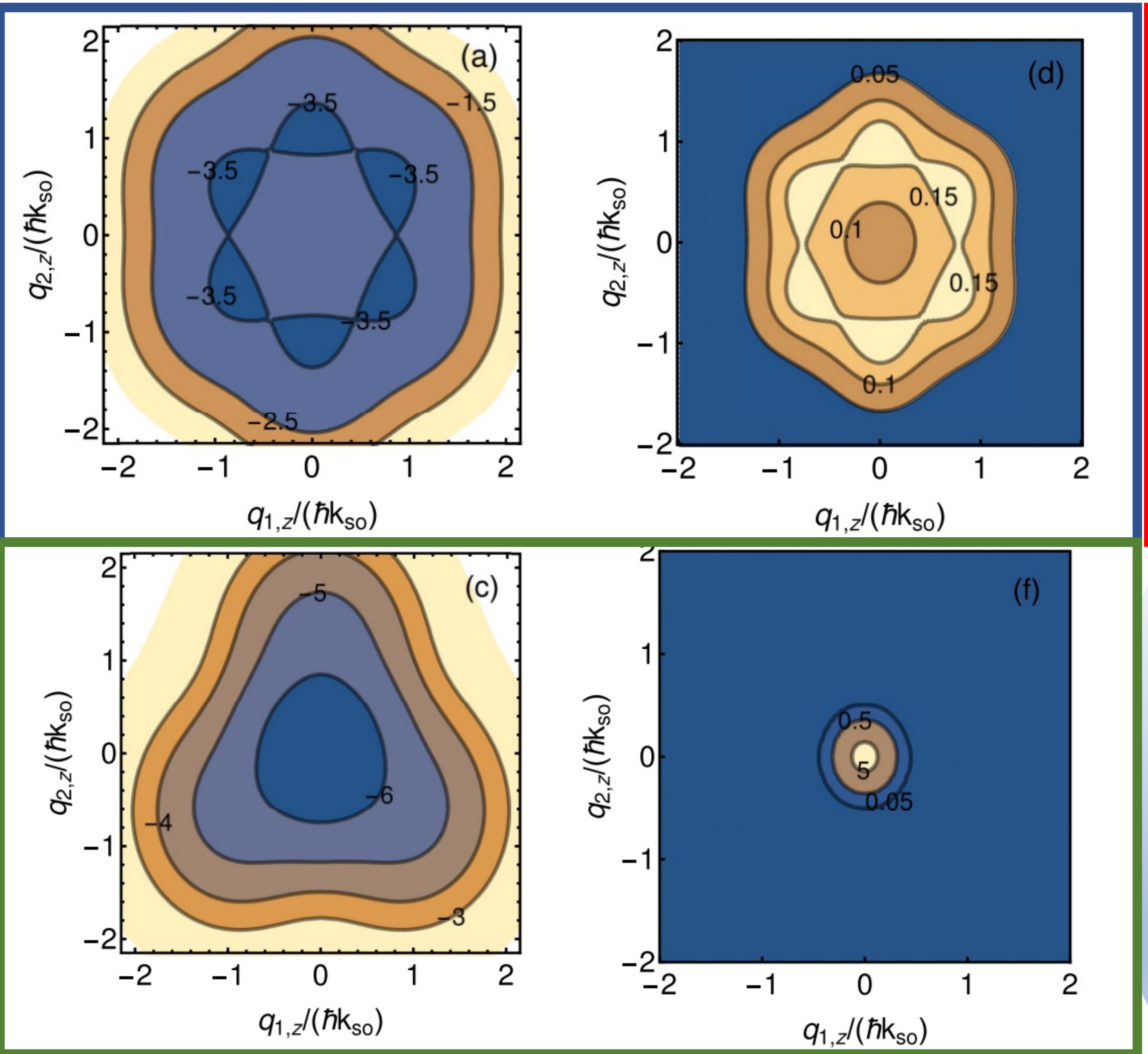
- The binding energy is the largest near the highest degeneracy scattering threshold

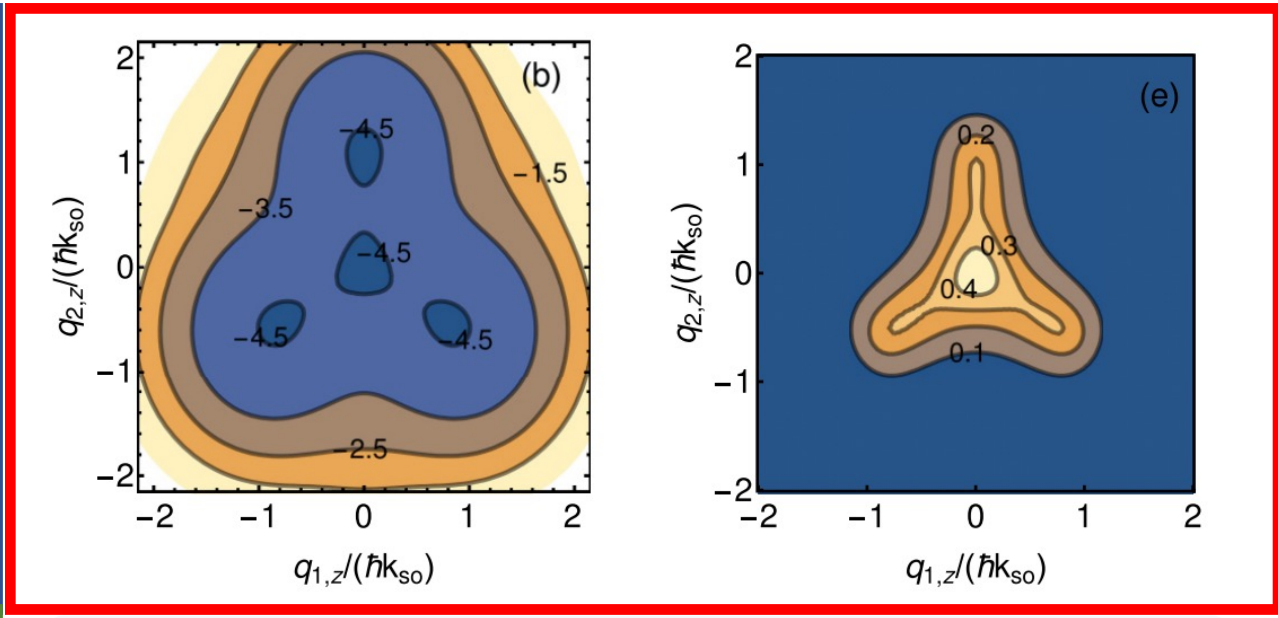
- The second largest binding near $\tilde{\delta} = 0$.



Q. Guan and D. Blume, PRX 8, 021057 (2018)

Three-Boson System with 1D SOC---Structural Property





The momentum space structure of the trimer follows that of the scattering threshold. More peaks in momentum space means stronger coupling effects!

Q. Guan and D. Blume, PRA 100, 042708 (2019)

Three-Boson System with 1D SOC--- Summary

- A discrete radial scaling law exists in an enlarged parameter space and verified numerically.
- Due to broken Galilean invariance, the Hamiltonian of the relative d.o.f depends parametrically on the total COM momentum.
- To determine the atom dimer scattering threshold, the full COM momentum dependence of the dimer energy is mapped out.
- The strength of the binding energy is correlated to the degeneracy of state near the scattering threshold.
- The structure of the trimer in momentum space is highly correlated to that of the threshold states.

Two and Three-Body Systems with Synthetic Spin-Orbit Coupling

Qingze Guan

1.Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklahoma
2.Center for Quantum Research and Technology, The University of Oklahoma, Norman, Oklahoma
3. Department of Physics and Astronomy, Washington State University, Pullman, Washington

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Thanks !