SEARCH FOR STABLE STATES IN TWO-BODY EXCITATIONS OF THE HUBBARD MODEL

on the Honeycomb Lattice

30 JULY 2024 I PETAR SINILKOV I NRW-FAIR

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IN COLLABORATION WITH

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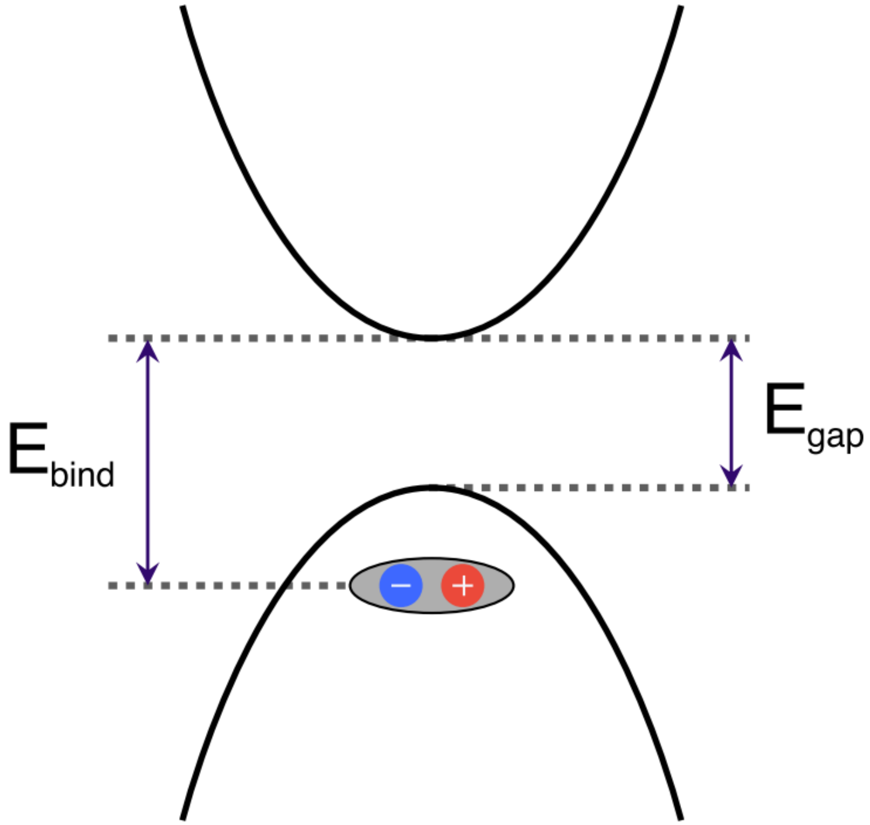
THOMAS LUU (FORSCHUNGSZENTRUM JÜLICH)

OUTLINE

EXCITON

- An exciton is a bound state of an electron and a hole
  - Bosonlike quasi-particle with a net charge zero
- Formed when the binding energy of the electron-hole pair is larger than the band gap
- Good candidates for the development of topologically protected qubits, switching devices, and heat exchangers



K. Wu et al., Physical Review Applied 2 (2014) 054013
S. K. Banerjee et al., IEEE Electron Device Letters 30 (2009) 158
S. Peotta et al., Phys. Rev. B 84 (2011) 184528

EXCITON

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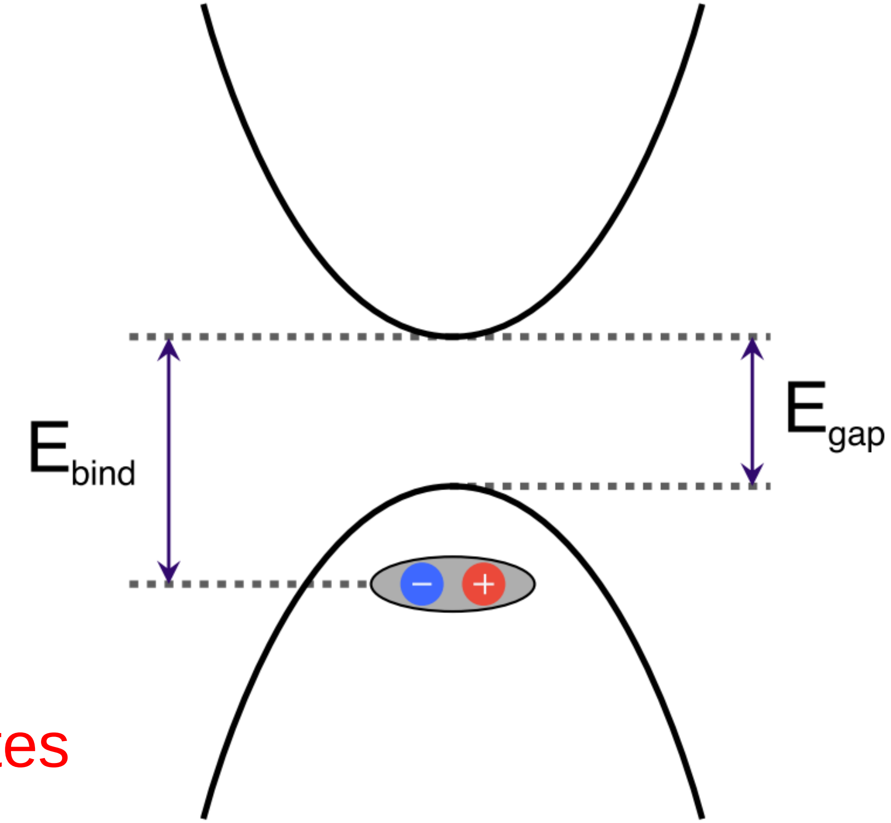

We need non-perturbative calculations for bound states

K. Wu et al., Physical Review Applied 2 (2014) 054013
S. K. Banerjee et al., IEEE Electron Device Letters 30 (2009) 158
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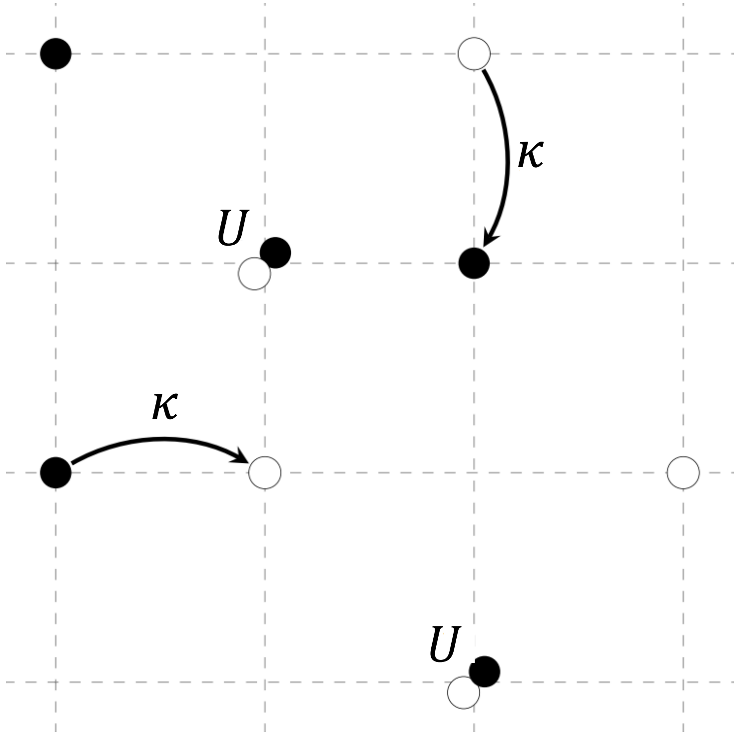
THE HUBBARD MODEL

$$H - \mu \cdot q = -\kappa \sum_{\langle xy \rangle} \left(p_x^\dagger p_y - h_x^\dagger h_y \right) + \frac{U}{2} \sum_x q_x^2 - \mu \sum_x q_x$$

- $p^\dagger, p$: creation/annihilation operators for particles
- $h^\dagger, h$: creation/annihilation operators for holes
- κ : hopping parameter
- U : on-site interaction
- $q_x = n_x^p - n_x^h \equiv p_x^\dagger p_x - h_x^\dagger h_x$: local charge
- μ : chemical potential



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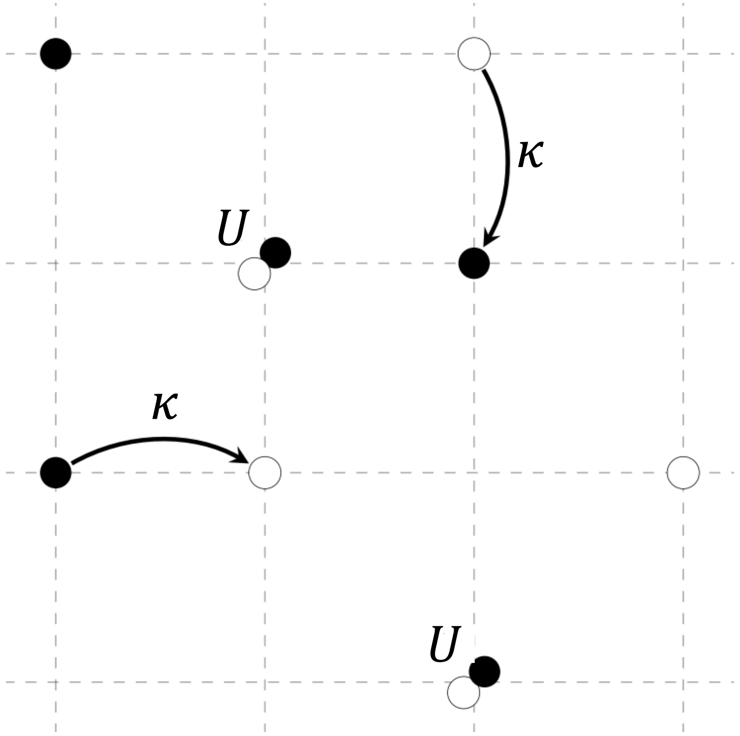


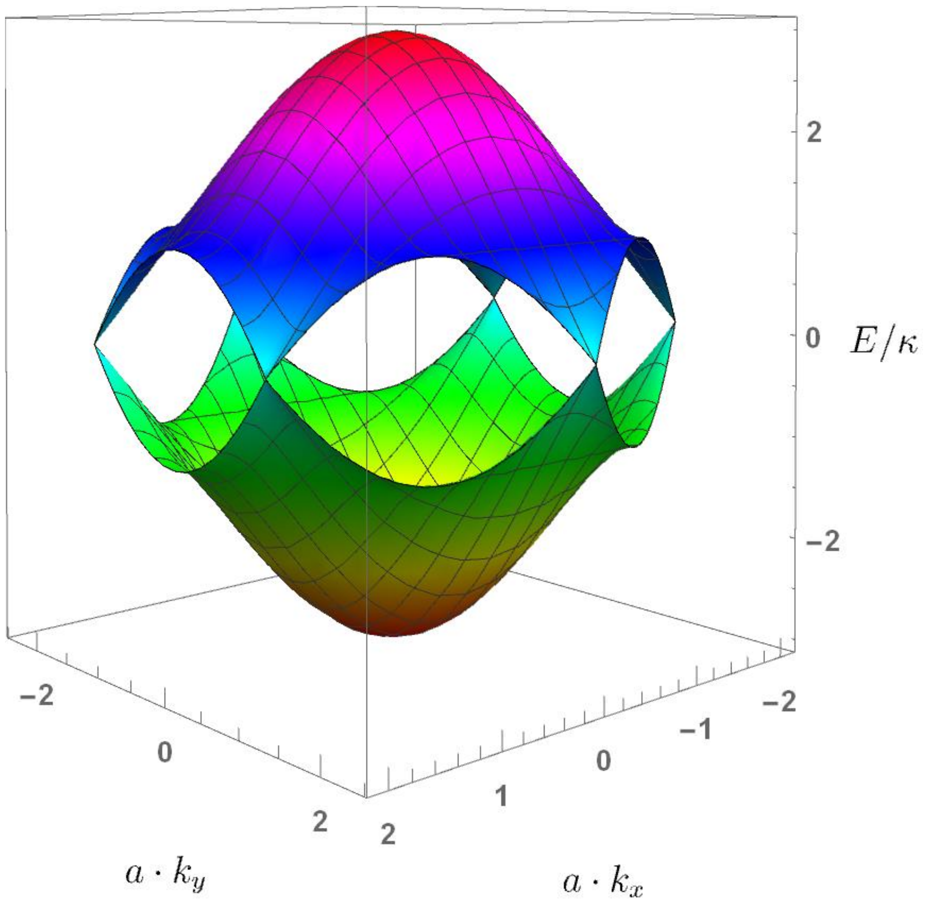
THE HUBBARD MODEL

Non-Interacting case

- An exact solution exists for non-interacting case at half-filling

$$E_{\vec{k}\pm} = \pm(-\kappa)\sqrt{3 + 2\left(\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) + \cos(\sqrt{3}k_y)\right)}$$

- It gives rise to a two-band structure
- We can calculate all multi-particle energies



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THE HUBBARD MODEL

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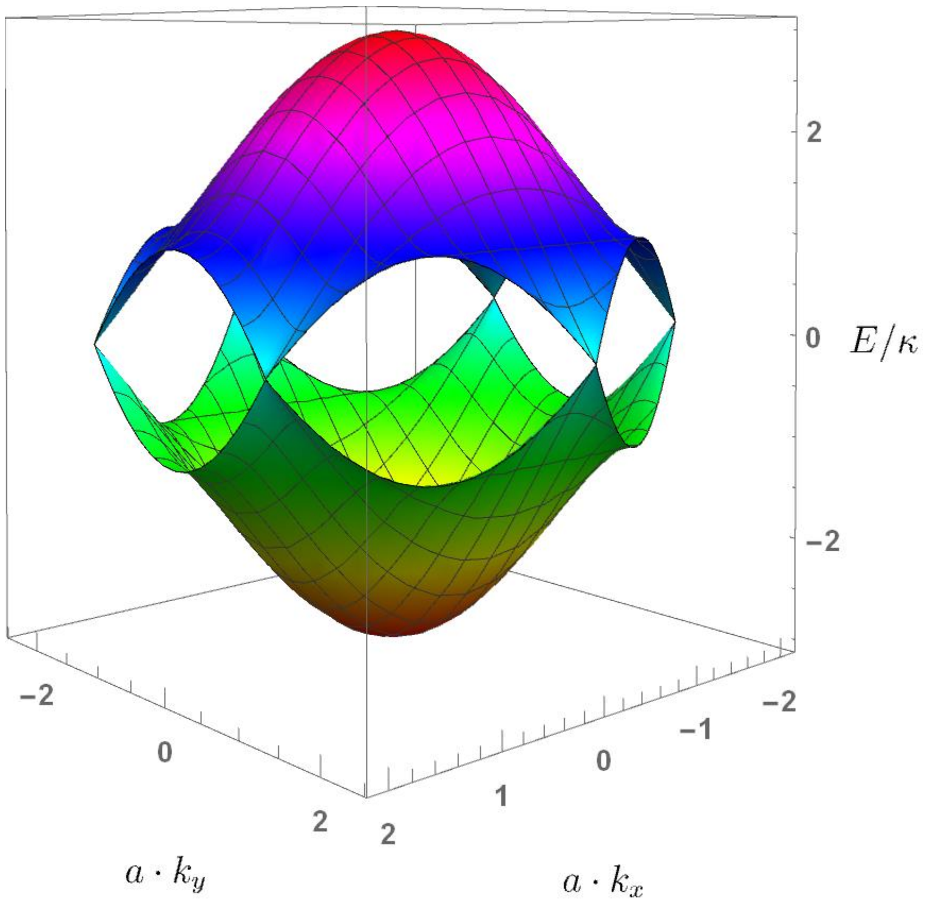
- We can calculate all multi-particle energies

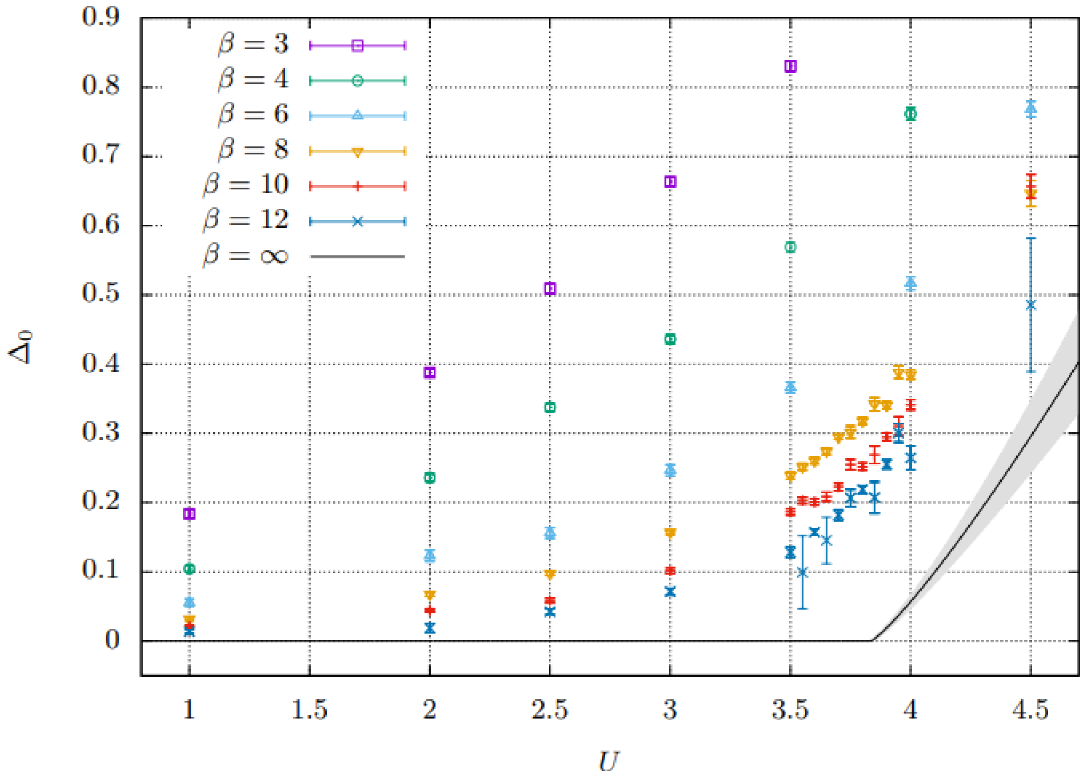
More interesting when we turn on interactions

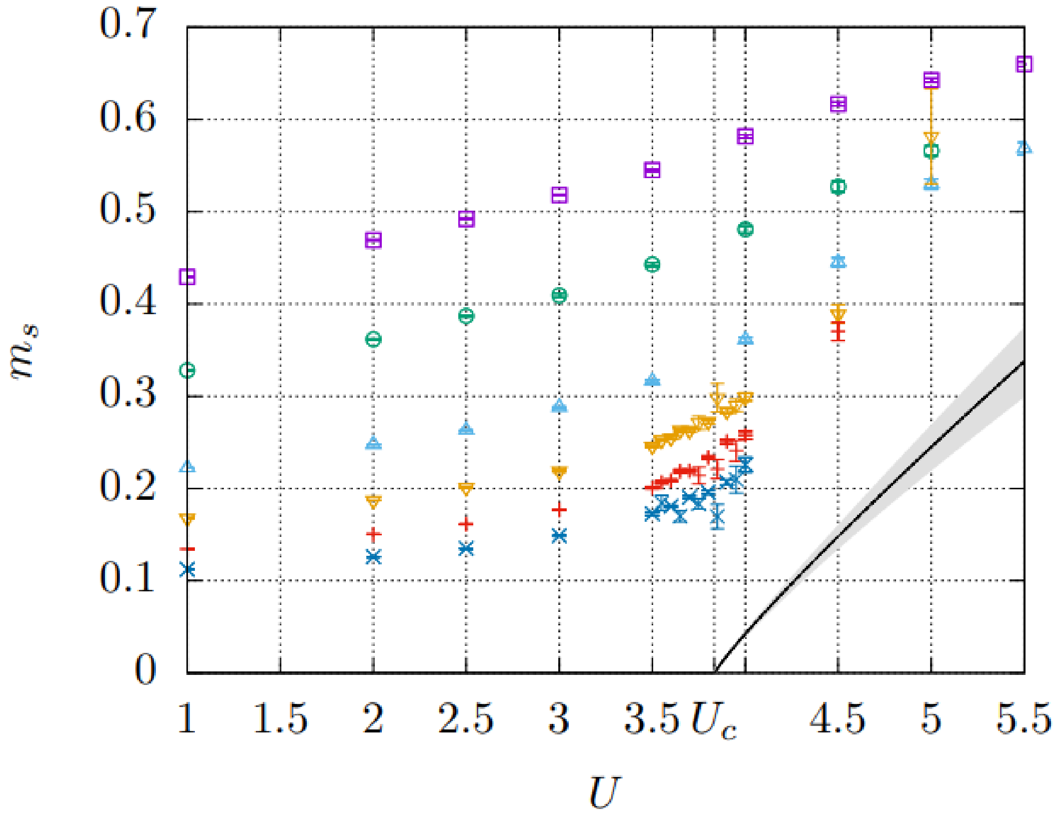


THE HUBBARD MODEL

One-body band gap

J. Ostmeyer et al., arXiv:2005.11112
J. Ostmeyer et al., Phys. Rev. B 102 (2020) 245105





One-body gap forms at $U_c \cong 3.835$

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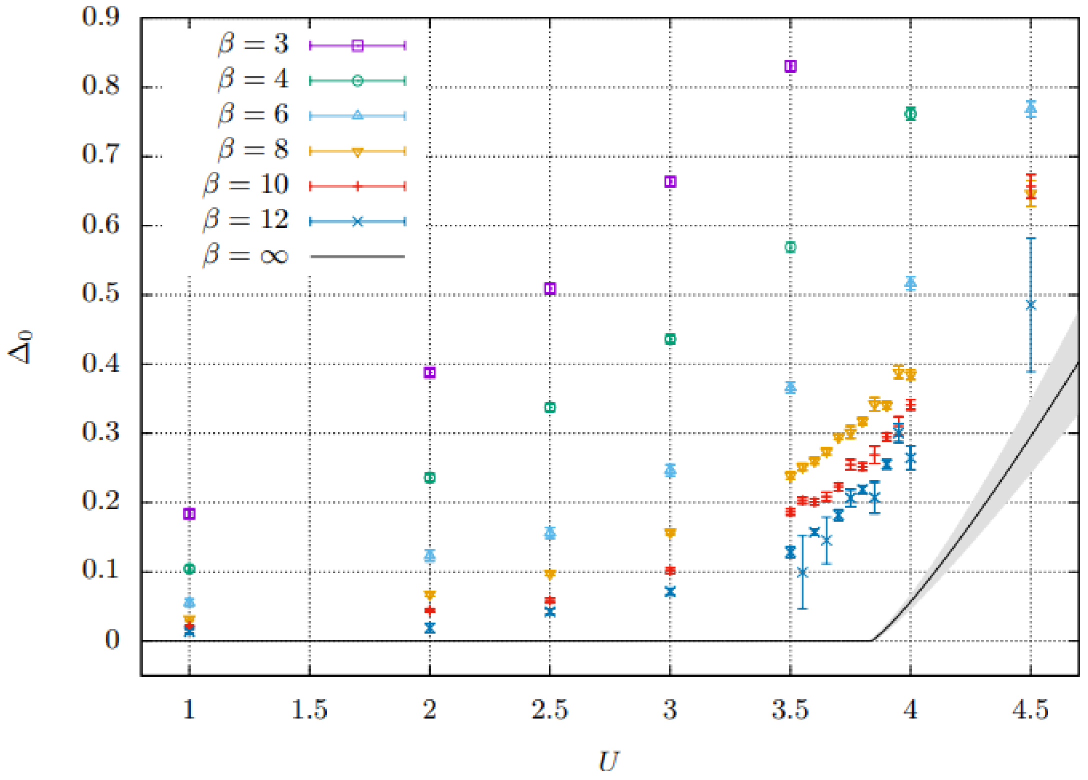

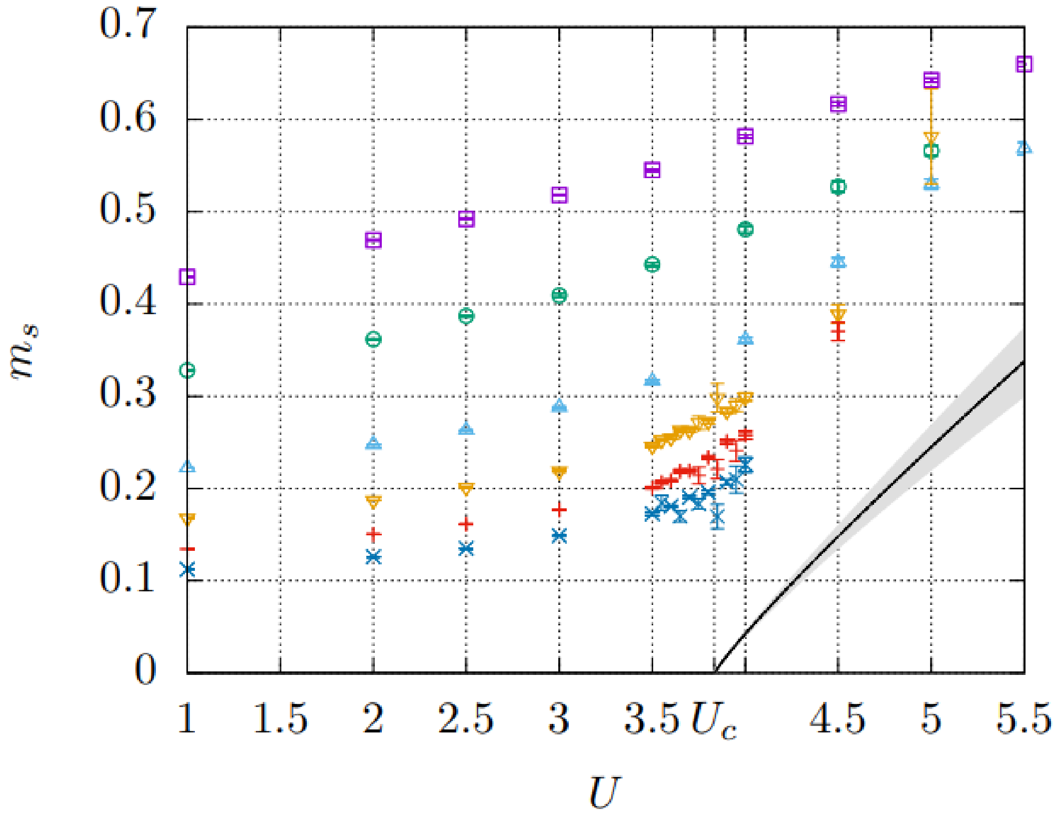

One-body gap forms at $U_c \cong 3.835$

What happens with two-body states?

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CORRELATION FUNCTIONS

Two-point correlation functions

$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \rangle$$

- The Hubbard model can have single-electron excitations, while QCD does not have single-quark excitations

$$I = 1/2, S = 1/2$$

	$S_z = 1/2$	$S_z = 1/2$
$I_z = 1/2$	$p^\dagger$	h
$I_z = -1/2$	$h^\dagger$	p

- We can construct from these one-body operators all two-body operators

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CORRELATION FUNCTIONS

Two-body correlation functions

$I = 0, S = 0$

	$S_z = 0$
$I_z = 0$ $(Q = 0)$	$\frac{1}{2}(p_k p_l^\dagger + p_k^\dagger p_l + h_k h_l^\dagger + h_k^\dagger h_l)$

$I = 0, S = 1$

	$S_z = 1$	$S_z = 0$	$S_z = -1$
$I_z = 0$ $(Q = 0)$	$\frac{1}{\sqrt{2}}(p_k^\dagger h_l^\dagger - h_k^\dagger p_l^\dagger)$	$\frac{1}{2}(p_k p_l^\dagger - p_k^\dagger p_l + h_k h_l^\dagger - h_k^\dagger h_l)$	$\frac{1}{\sqrt{2}}(p_k h_l - h_k p_l)$

$I = 1, S = 0$

	$S_z = 0$
$I_z = 1$ $(Q = 2)$	$\frac{1}{\sqrt{2}}(p_k^\dagger h_l - h_k p_l^\dagger)$
$I_z = 0$ $(Q = 0)$	$\frac{1}{2}(p_k^\dagger p_l - p_k p_l^\dagger + h_k h_l^\dagger - h_k^\dagger h_l)$
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$I = 1, S = 1$

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$I_z = 1$ $(Q = 2)$	$p_k^\dagger p_l^\dagger$	$\frac{1}{\sqrt{2}}(p_k^\dagger h_l + h_k p_l^\dagger)$	$h_k h_l$
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$I_z = -1$ $(Q = -2)$	$h_k^\dagger h_l^\dagger$	$\frac{1}{\sqrt{2}}(p_k h_l^\dagger + h_k^\dagger p_l)$	$p_k p_l$

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Do not measure channels with disconnected diagrams

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CORRELATION FUNCTIONS

Two-body correlation functions

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	$S_z = 0$
$I_z = 0$ ($Q = 0$)	$\cancel{\frac{1}{2}(p_k p_l^\dagger + p_k^\dagger p_l + h_k h_l^\dagger + h_k^\dagger h_l)}$

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Results in these channels

CORRELATION FUNCTIONS

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$I = 1, S = 0$

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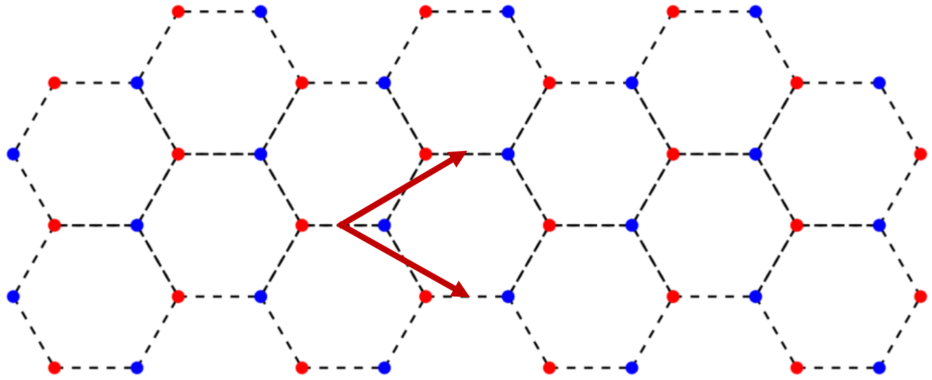
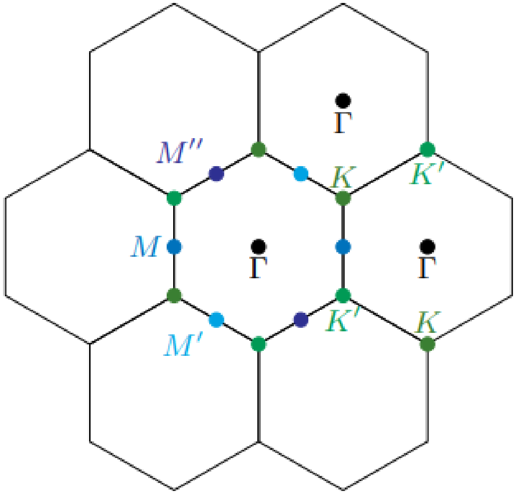
We expect $I_z = \pm 1$ to be repulsive while $I_z = 0$ to be attractive

HONEYCOMB LATTICE

- Bipartite lattice
  - Two triangular lattices
  - Every lattice site has a neighbor from the other sublattice
- We work in momentum space
  - Momenta modes of interest are – Γ, K, K’, M, M’, M’’
- Only the first Brillouin zone (BZ) is of interest because everything outside can be modded back.





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HONEYCOMB LATTICE

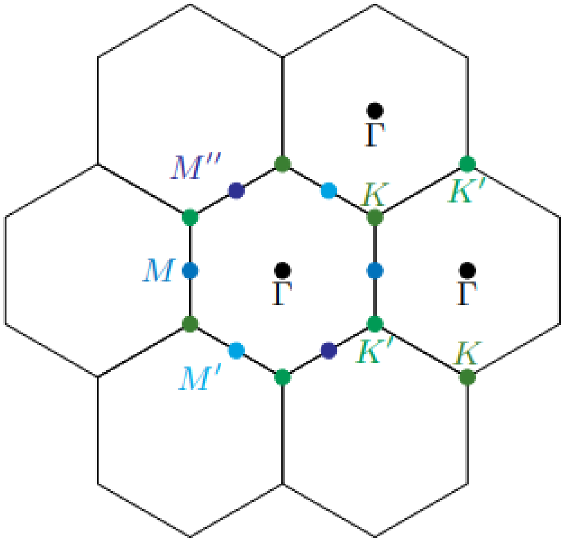
Symmetries

Must account the structure of the lattice

- Possible to leave the first BZ when adding momenta
- Work with total momentum P and relative momentum p instead

$$k, l \rightarrow P, p$$

- Total momentum is conserved
  - with total momentum P construct shells of relative momentum in irreps of the little group (allowing for umklapp)



K + K' = Γ
K + K = K'
K' + K' = K

DATA ANALYSIS

- Analysis is done at
  - Total momentum Γ, K and source/sink momenta K, K’
  - Lattice size - (3,3)
  - U = 3.0 and U = 4.0
  - $\beta \ = \ 8.0$
- We are not fitting an exponent because we leverage the symmetry of the correlators

$$f_{1/2}(t) = \sum_n A_n \, cosh\left(E_n^{1/2}(t - \frac{\beta}{2})\right)$$

- Calculate the energy shift

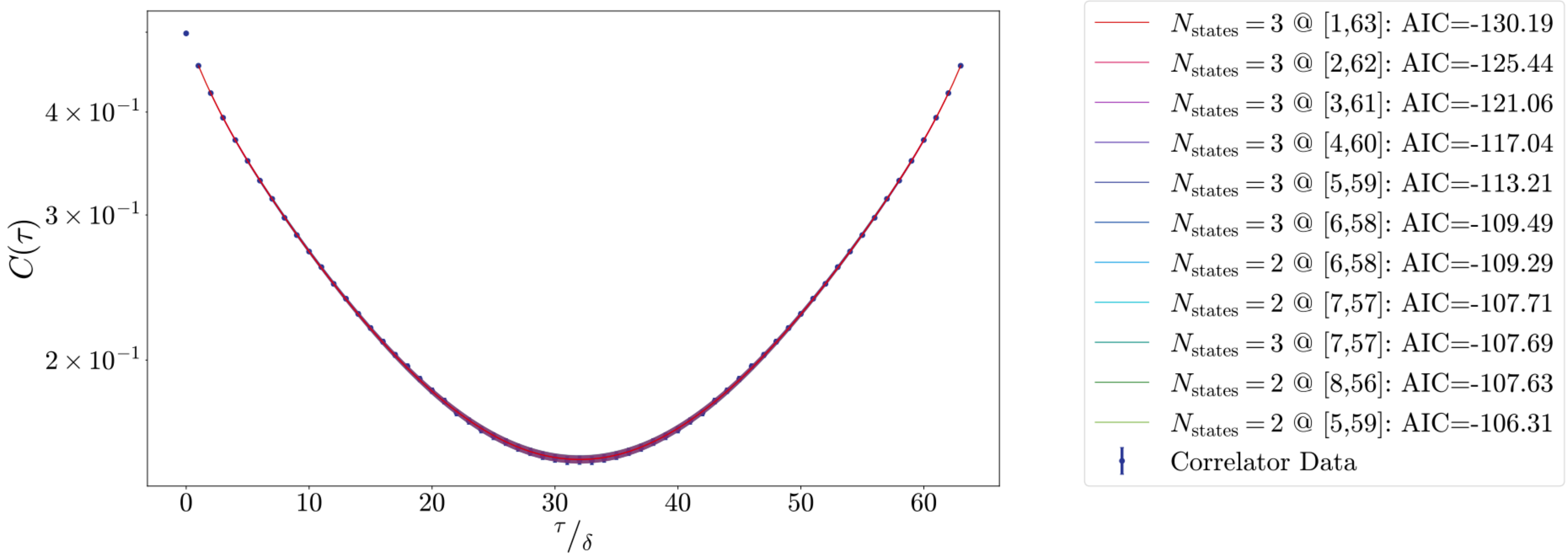
$$\Delta E = E^2 \ - 2E^1$$

- Extrapolate to the continuum limit $N_t \ \rightarrow \infty$
- Repeat for every channel
- Repeat for all available irreducible representations (Only A1 results presented)

K + K’ = Γ
K + K = K’
K’ + K’ = K

RESULTS

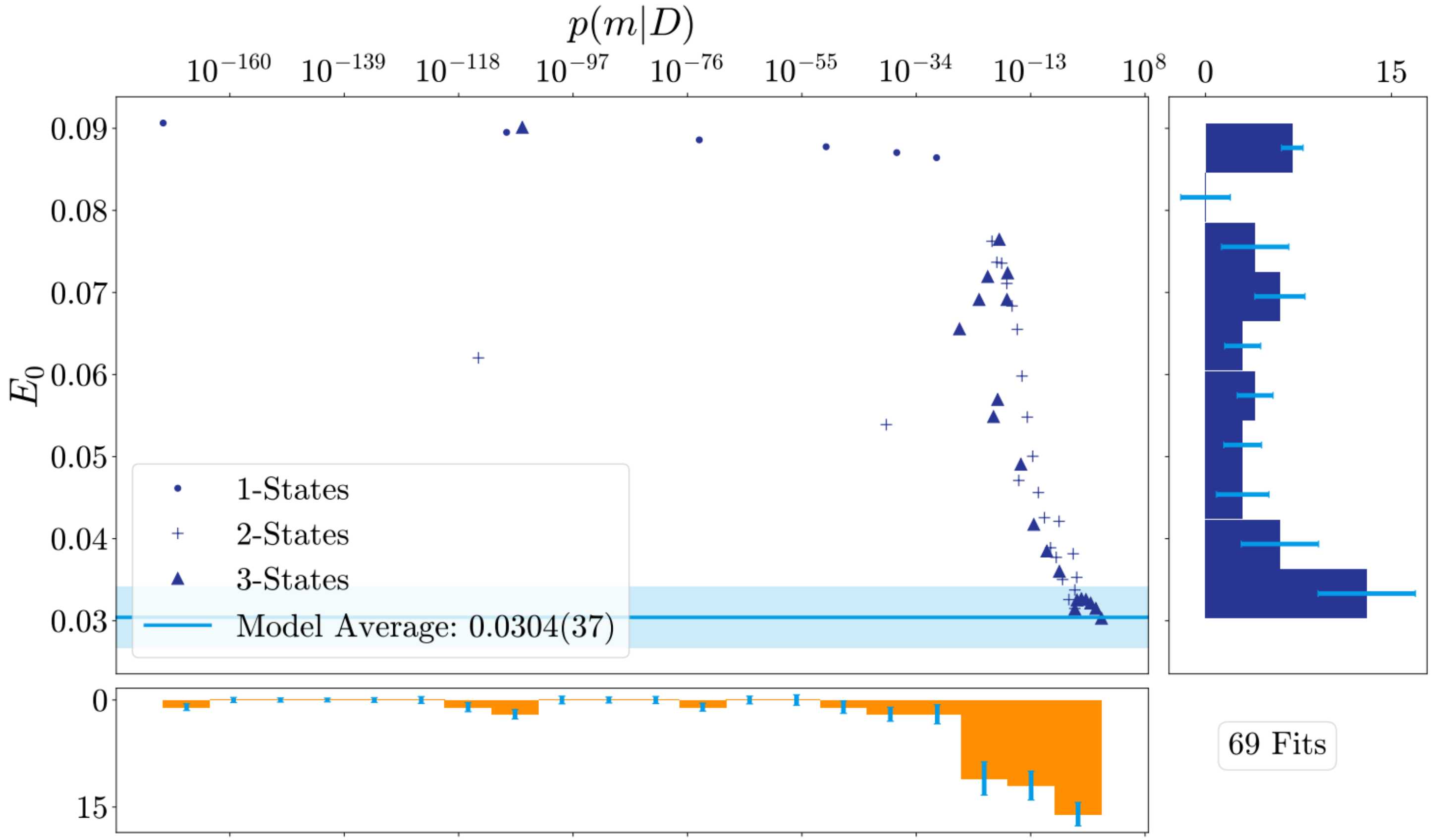
One-Body Correlation Function



The correlator is exceptionally flat!

RESULTS

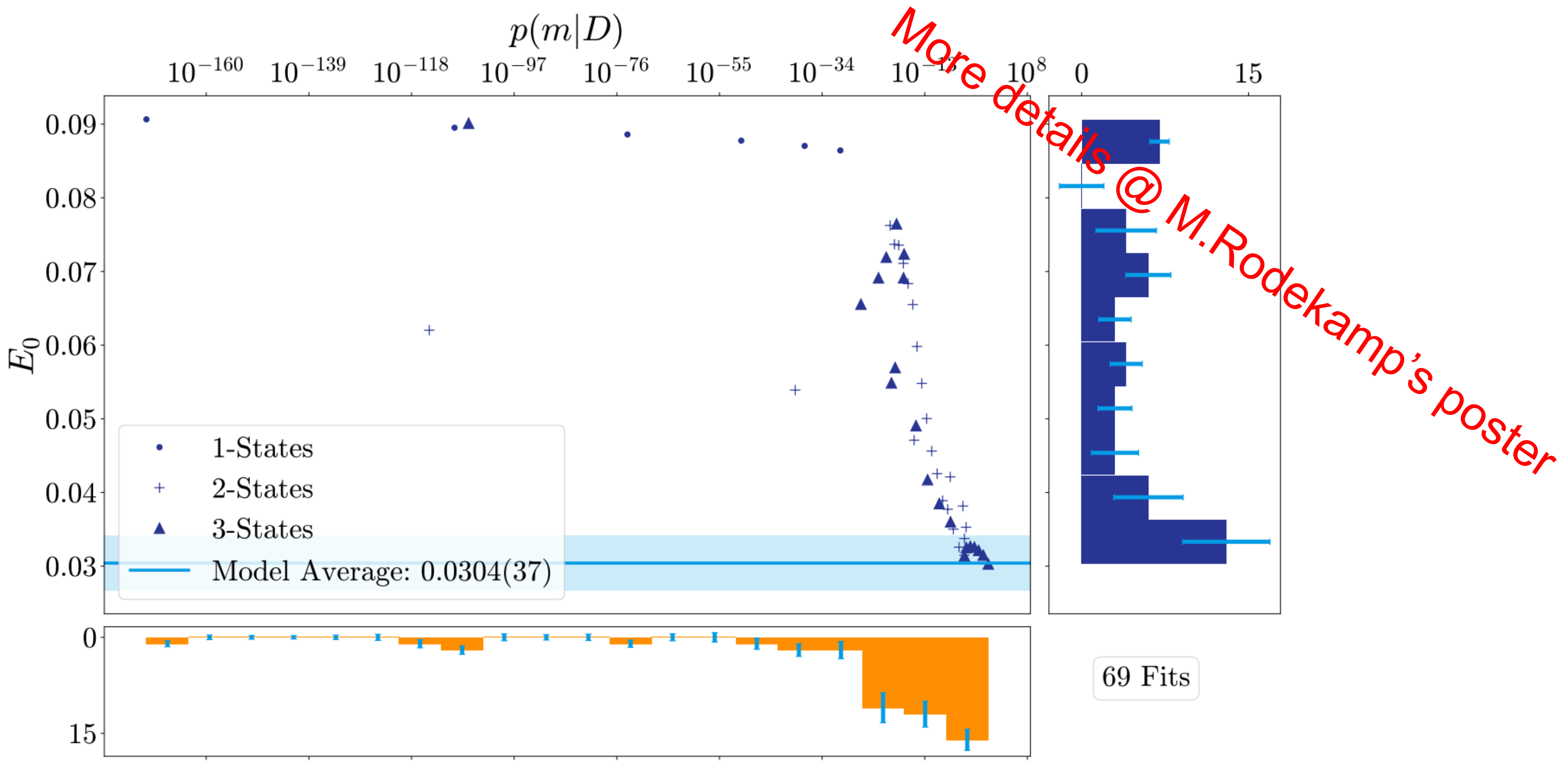
One-Body Correlation Function



Stability plot illustrating the Model Averaging

RESULTS

One-Body Correlation Function



Stability plot illustrating the Model Averaging

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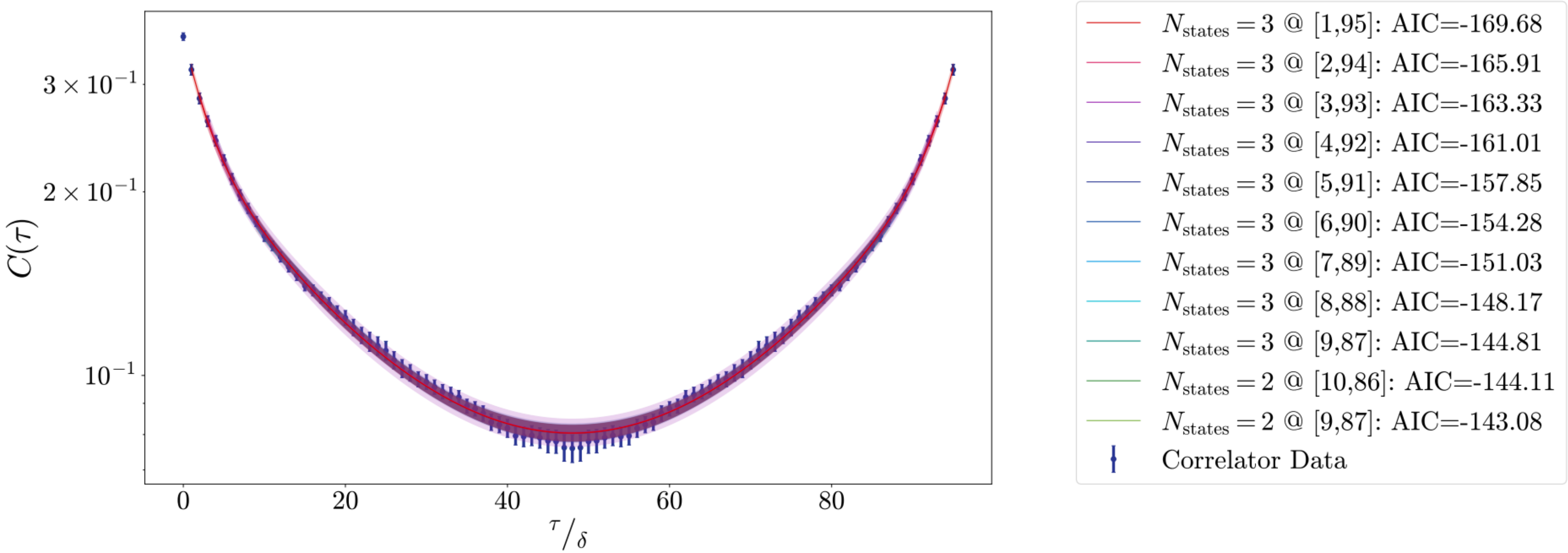
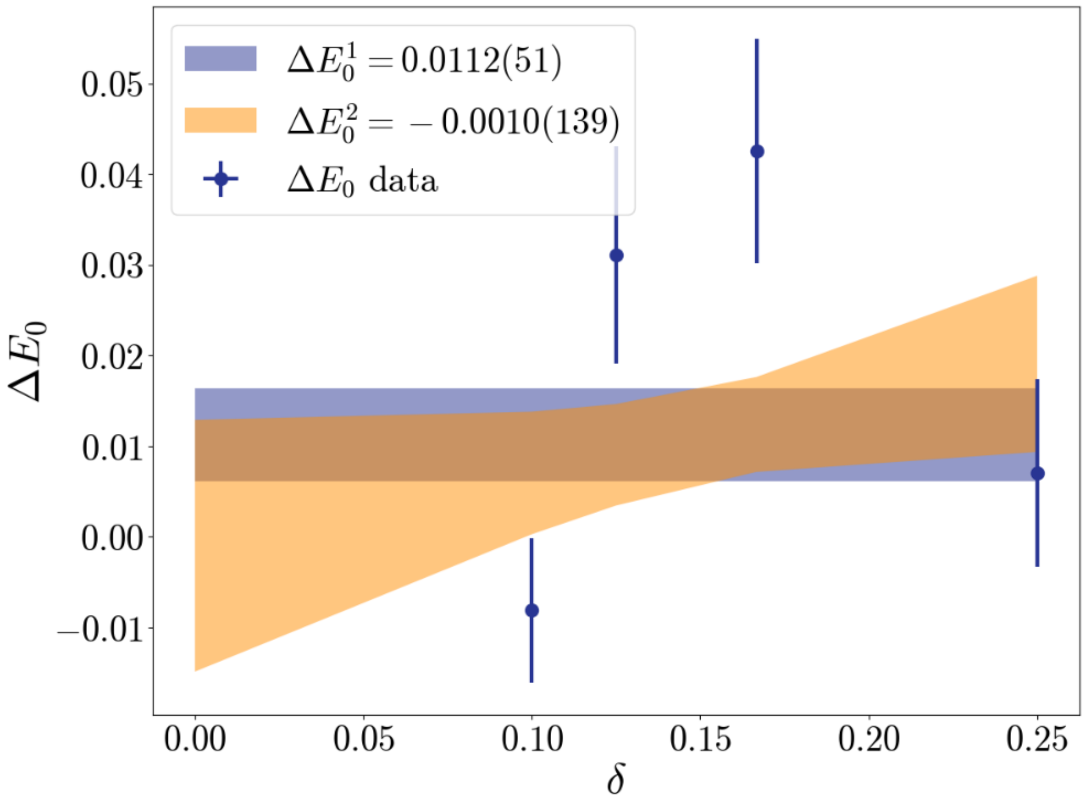


$$I = 1, S = 1; I_z = 0, S_z = 1 \ (U = 3.0)$$

$$E_0 = 0.093(11)$$

RESULTS

Continuum Limit U=3.0 @ P=Γ



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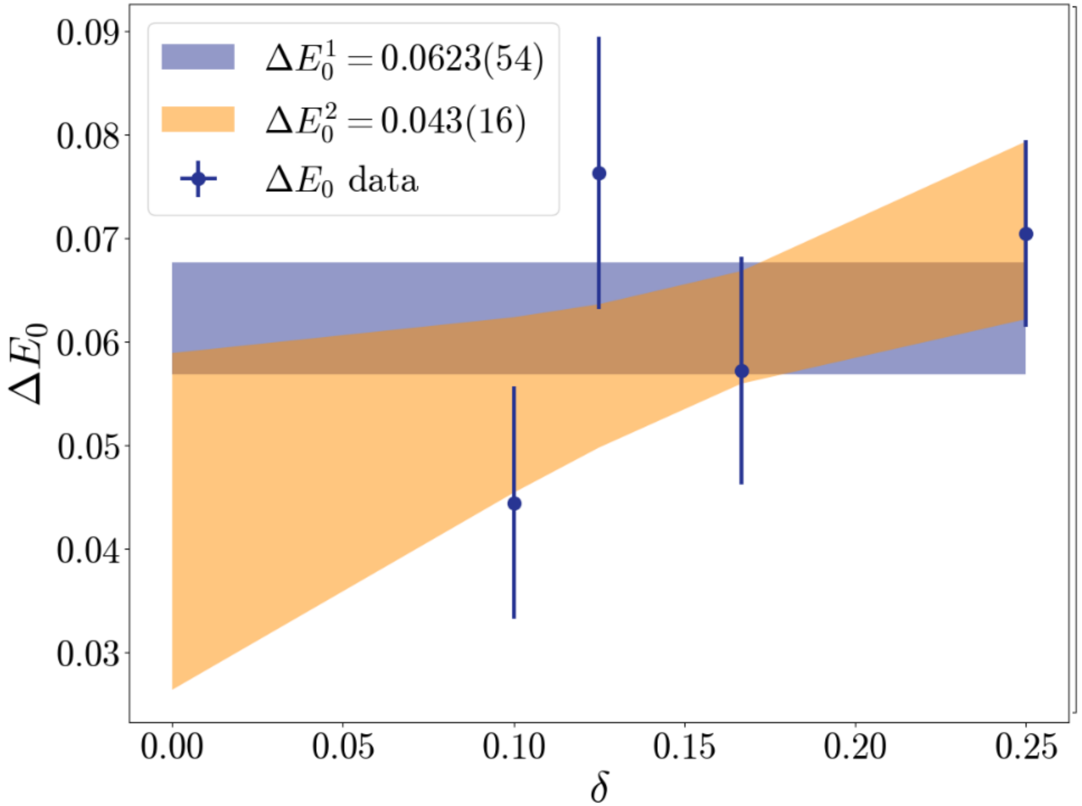

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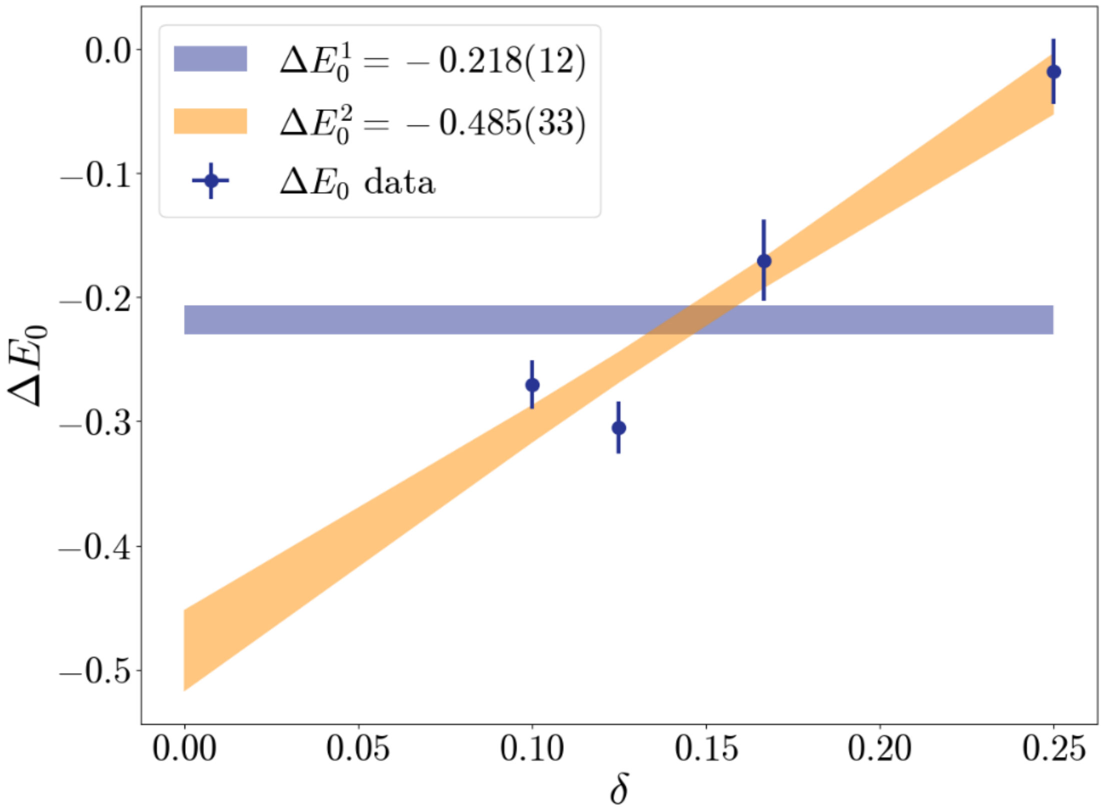
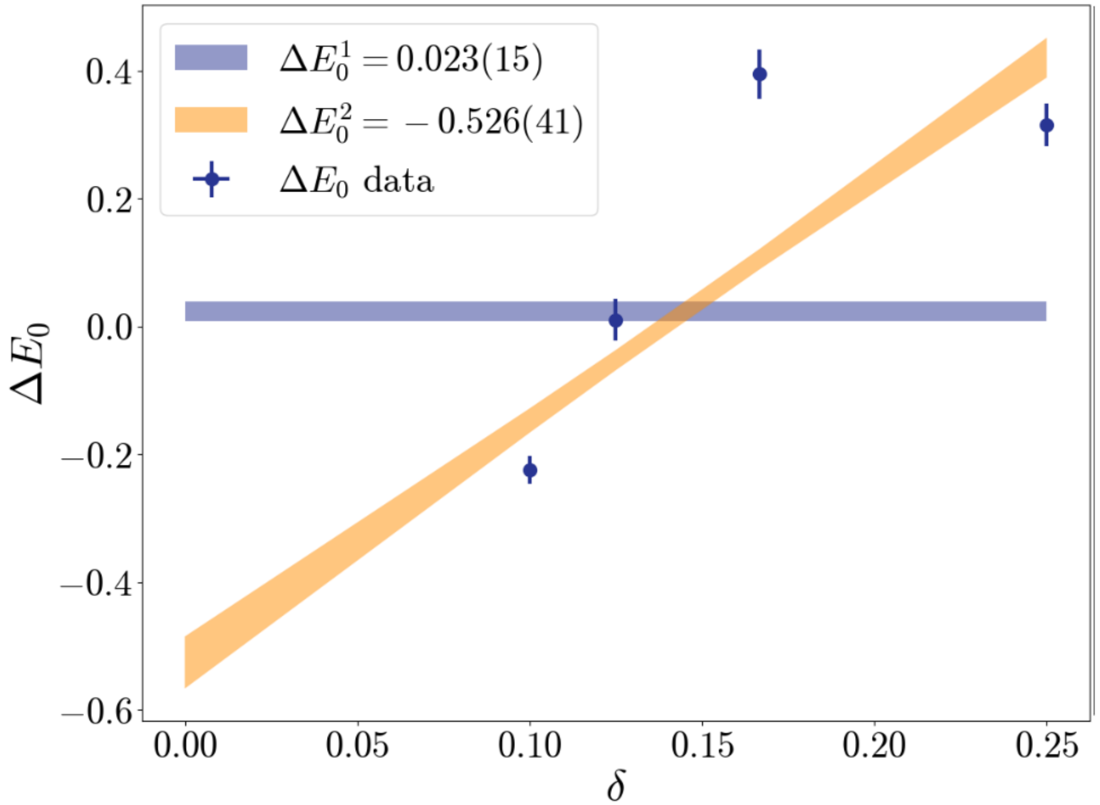
RESULTS

Continuum Limit U=4.0 @ P=Γ



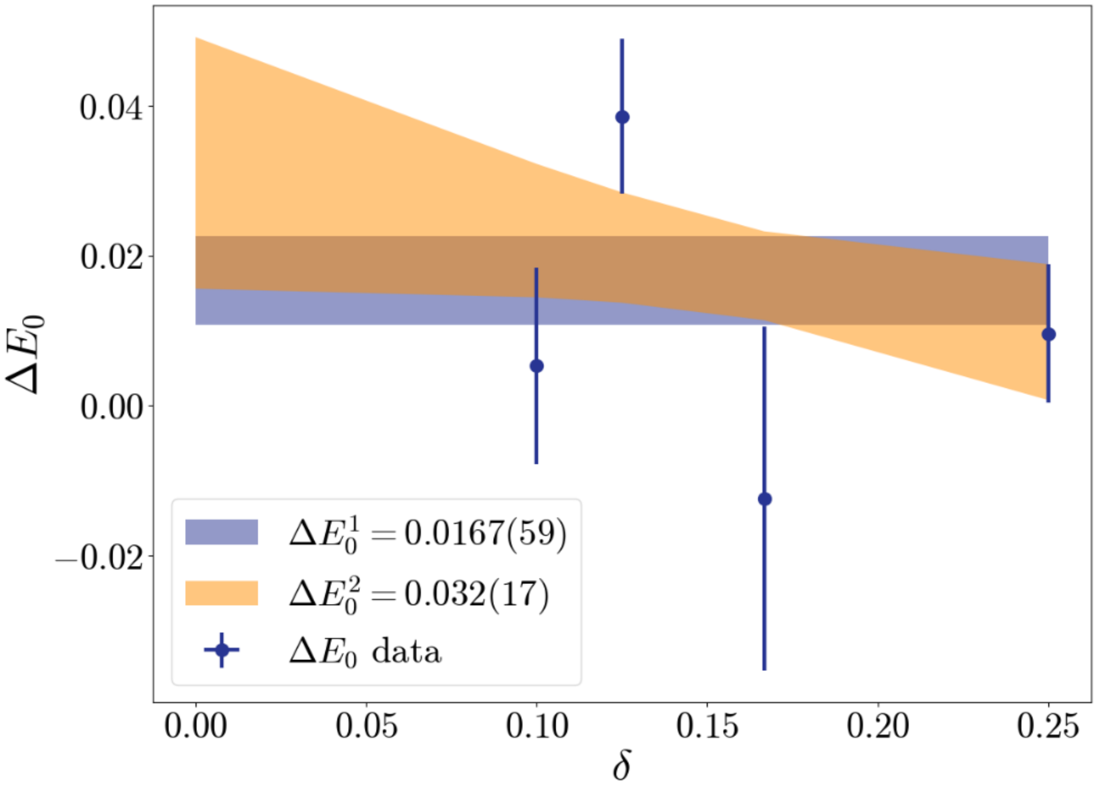
$I = 1, S = 1; I_z = 0, S_z = 1\ (U = 4.0)$



$I = 1, S = 1; I_z = 1, S_z = 1\ (U = 4.0)$

RESULTS

Continuum Limit U=3.0 @ P=K



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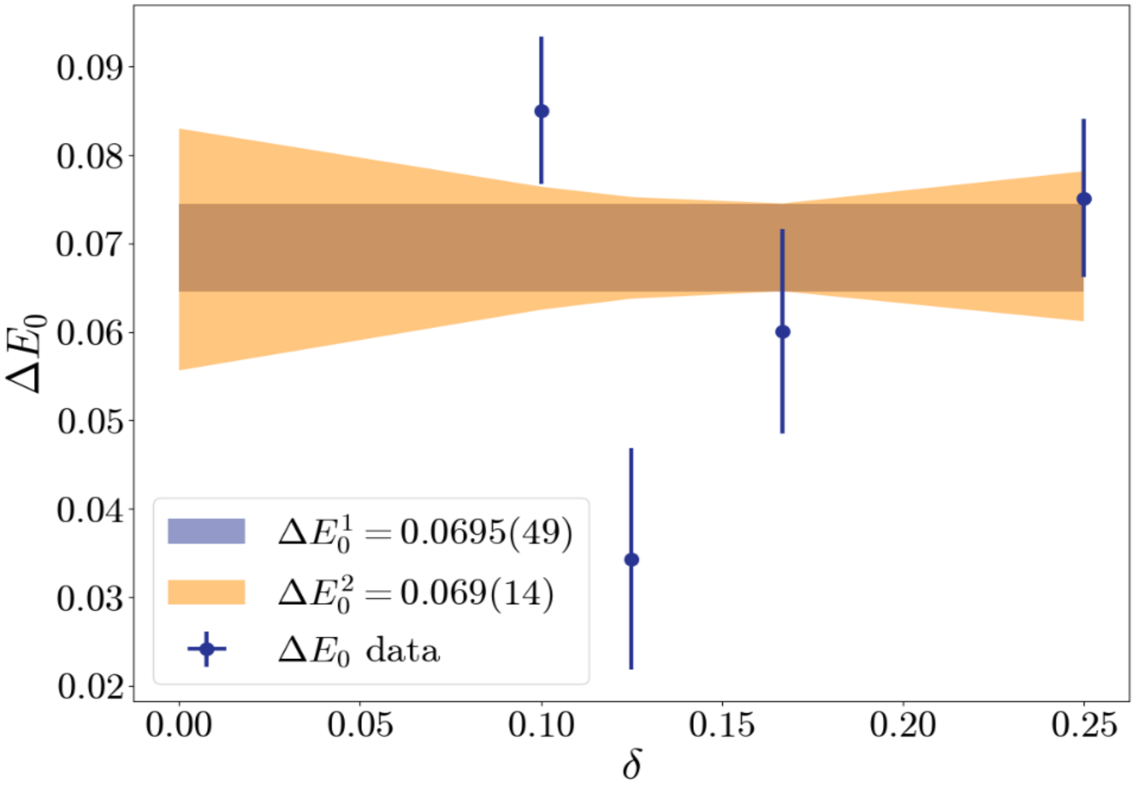

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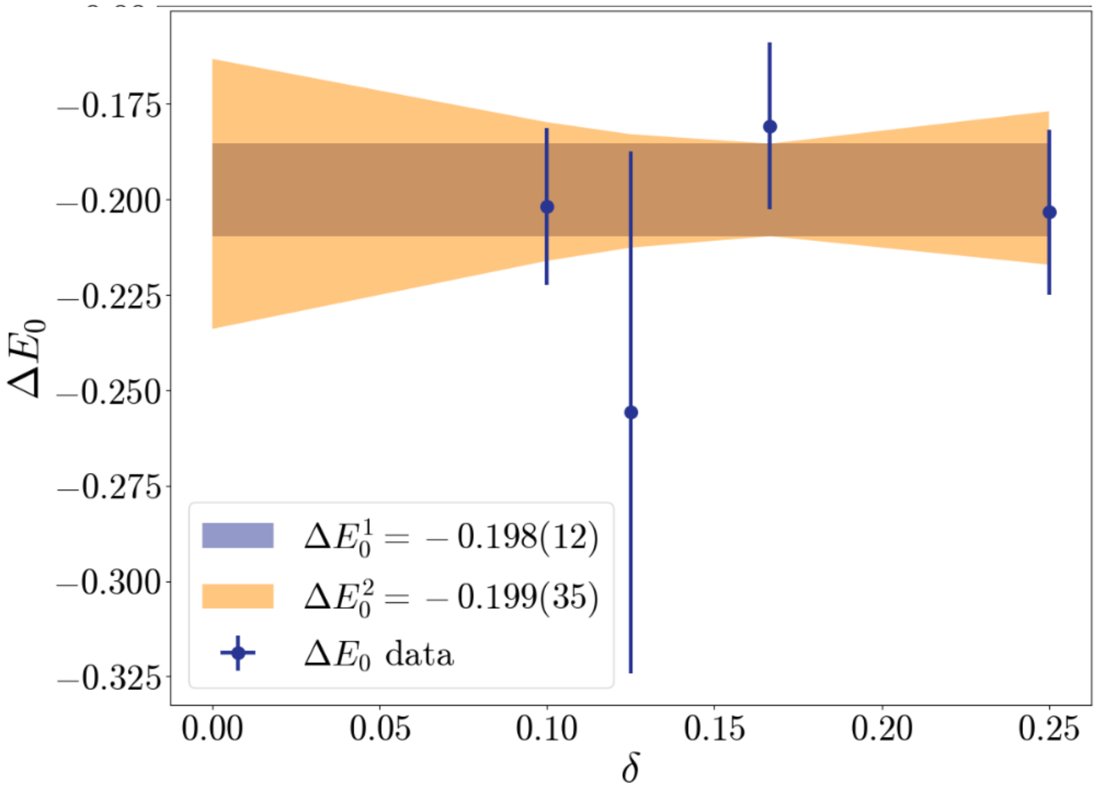

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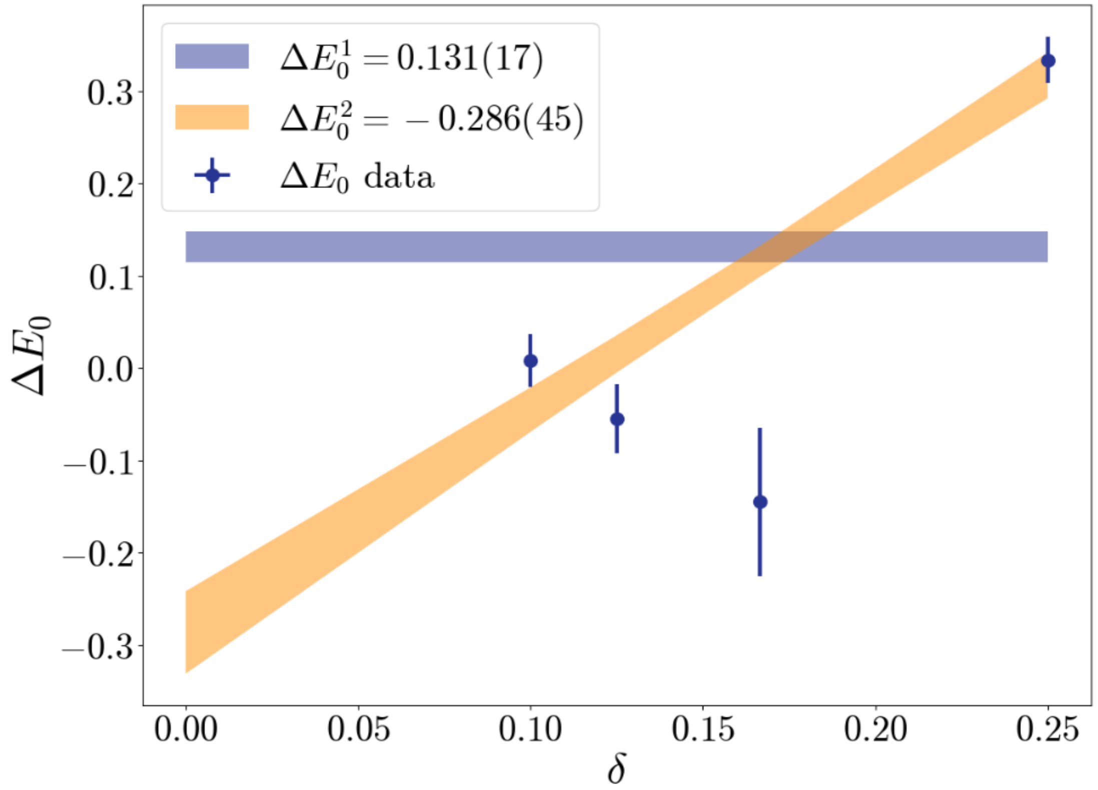

$I = 1, S = 1; I_z = 1, S_z = 1\ (U = 4.0)$

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SUMMARY

Outlook

What did we find?

As expected, we found that the attractive channel has smaller energy shift than the repulsive one.

Found positive energy shift at $U = 3.0$ in the channel with non-zero net charge at both total momenta.

Found positive or close to zero energy shift at $U = 3.0$ in the channel with zero net charge at both total momenta.

Negative or close to zero energy shift at $U = 4.0$ in the channel with non-zero net charge at both total momenta.

Negative zero energy shift at $U = 4.0$ in the channel with zero net charge at both total momenta. Possible bound state?

SUMMARY

Outlook

What did we find?

What does the future hold?

Generate ensembles, so we can reach the three limits simultaneously.

Add more data points to the extrapolations

Scan over U to get $\Delta E_0(U)$

Perform simulations at non-zero chemical potential $(\mu \neq 0)$

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