Strong coupling ansatz for the 1D Fermi gas in a harmonic potential

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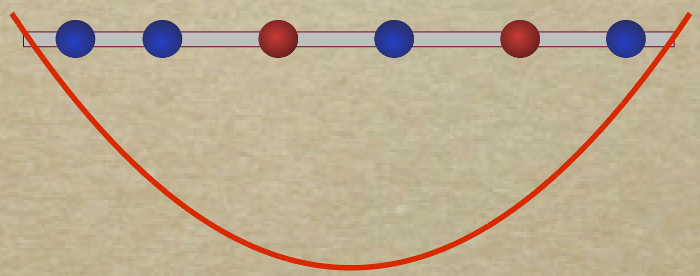
Two fundamental quantum systems

- Particles in **one dimension** is a fundamental problem of strongly correlated systems
  - *Interactions are enhanced due to the particles' restricted motion*
  - *Special role played by particle statistics*
- Many such systems amenable to exact solutions, such as Bethe ansatz



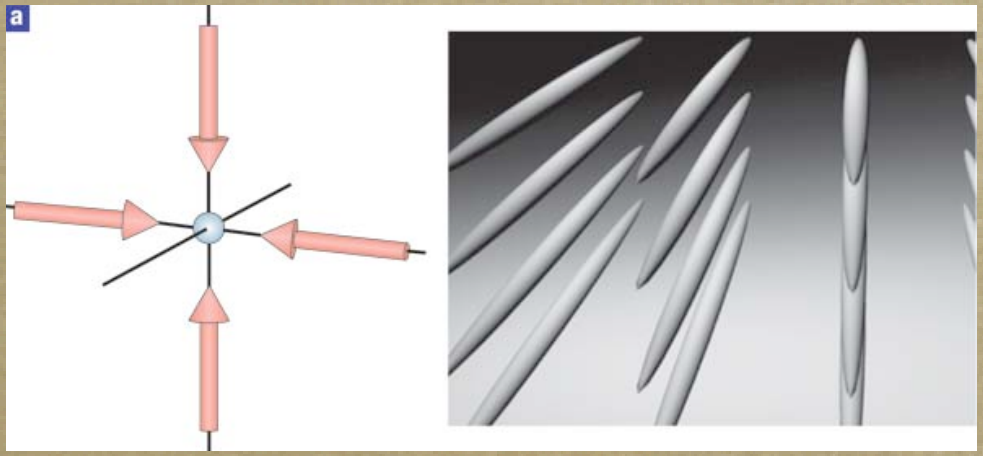
- The **harmonic oscillator** is a fundamental model of quantum physics
  - *In the absence of interactions, we know the exact ground state*
  - *No Bethe-ansatz solution for 1D fermions in a harmonic potential*

Model

- Two species (spins) of fermions with short-range interactions

$$\mathcal{H} = \sum_{i=0}^{N} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right] + g \sum_{i<j} \delta(x_i - x_j)$$

- Consider a single tube in an optical lattice



At low collision energies, the 3D interactions become effectively 1D:

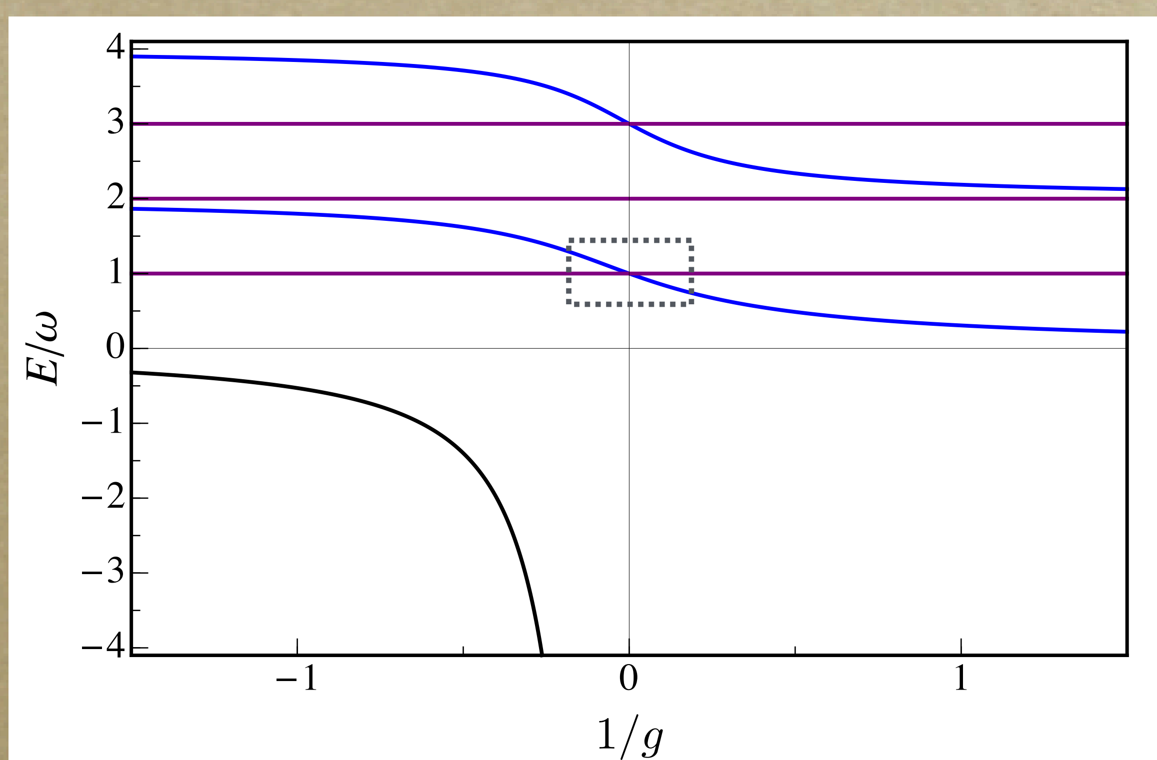
$$g = \frac{2\sqrt{2}\hbar^2}{m l_\perp} \left(\frac{\sqrt{2} l_\perp}{a} - \zeta(1/2) \right)^{-1}$$

Olshanii PRL 1998

Ultracold fermions in Heidelberg

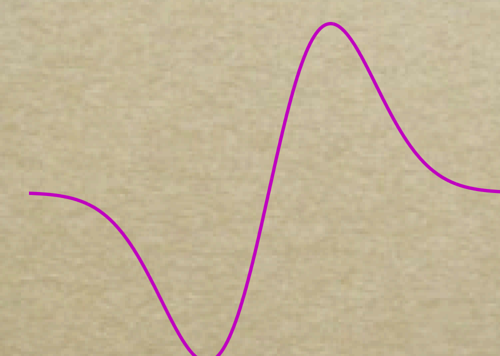
The 1D harmonic oscillator was realized in a recent series of experiments with two-component fermions in the group of S. Jochim

- *Fermionization of two distinguishable fermions* Zürn et al, PRL 2012

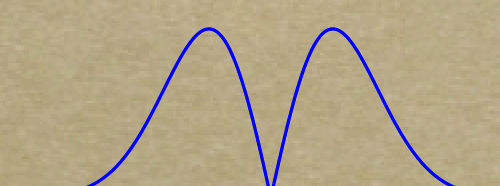


Exact solution: Busch et al, Foundations of Physics 1998

Wavefunctions in the Tonks-Girardeau limit:



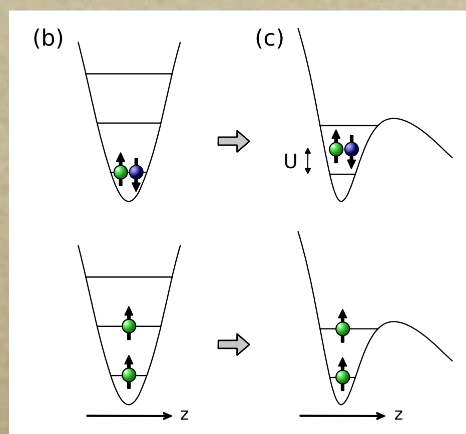
$x_{01} e^{-(x_0^2+x_1^2)/2}$



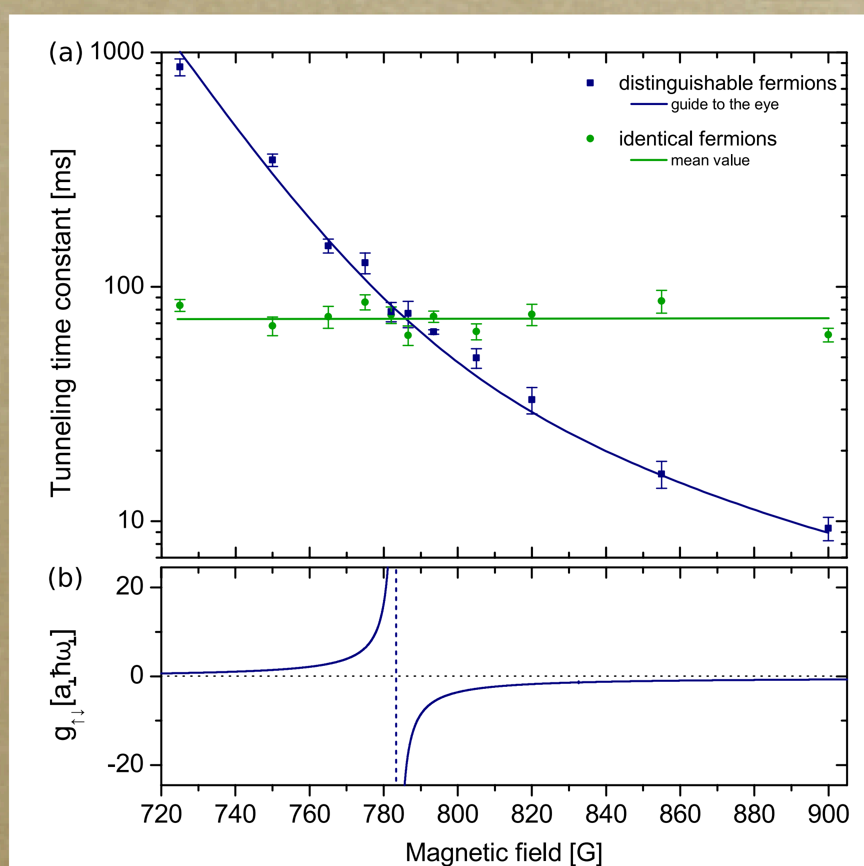
$|x_{01}| e^{-(x_0^2+x_1^2)/2}$

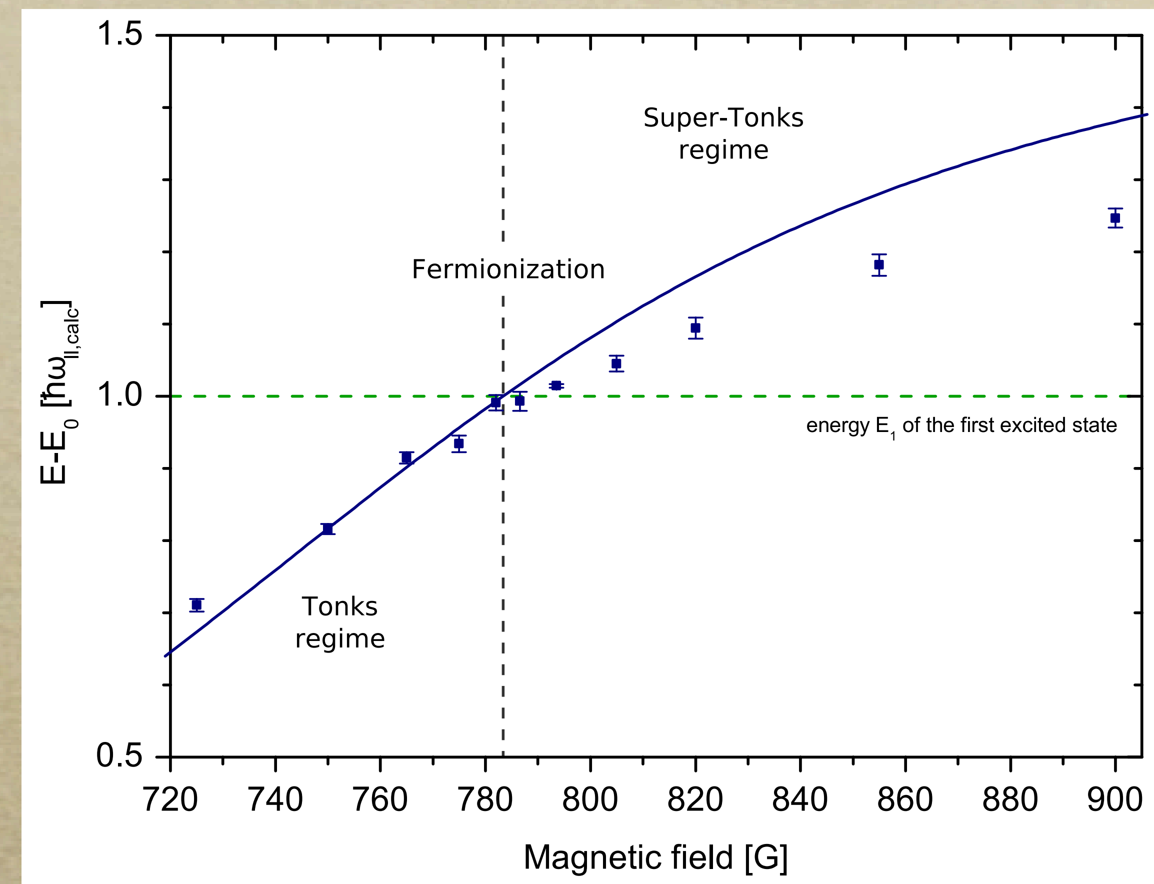
Ultracold fermions in Heidelberg

Tunneling experiment:



Zürn et al, PRL 2012





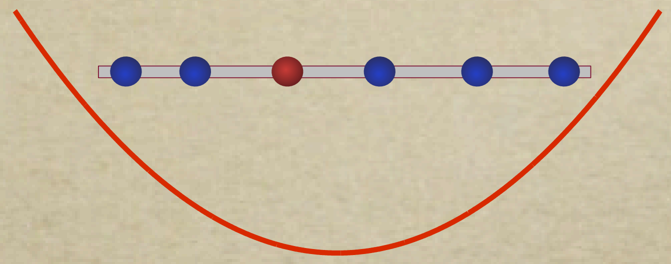
So far experiments with a single impurity and up to 5 majority atoms

Wentz et al, Science 2013

The single impurity problem

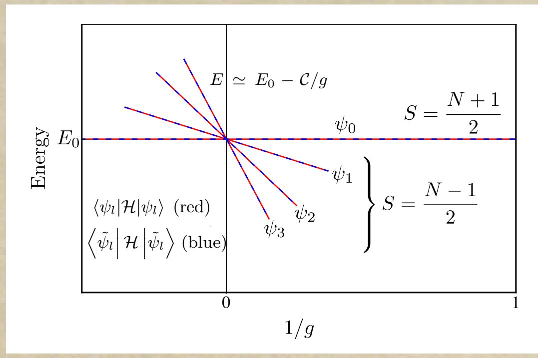
Inspired by the experiment, we focus on the

- *single impurity problem*
- *in a 1D geometry*
- *in an external harmonic potential*
- *in the vicinity of the Tonks-Girardeau limit of infinite repulsion*



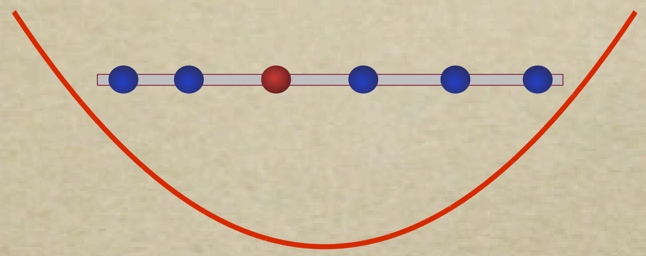
We show that this problem can be solved essentially exactly for any number of majority particles

The Tonks-Girardeau limit



For *N* spin-up fermions and *1* spin-down fermion there are *N+1* degenerate wavefunctions in the TG limit

- *# of ways to order the impenetrable particles*

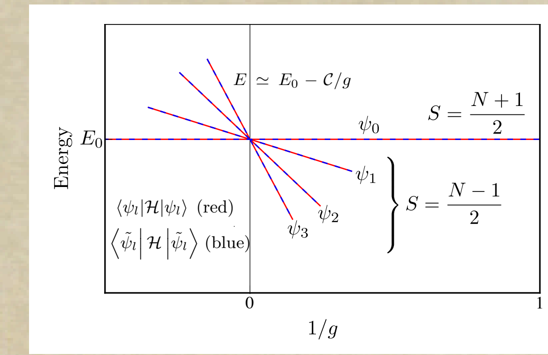


- *# of degenerate wavefunctions which are everywhere proportional to the fermionized wavefunction:*

$$\psi_0(\mathbf{x}) = \mathcal{N}_N \left(\prod_{0 \leq i < j \leq N} x_{ij} \right) e^{-\sum_{k=0}^{N} x_k^2/2}$$

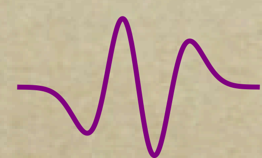
- *Such wavefunctions all have the same kinetic energy and vanishing interaction energy*

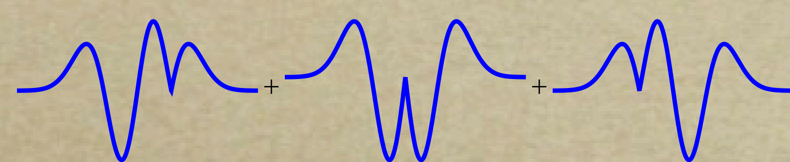
Basis functions for an <u>impurity</u> in the TG limit

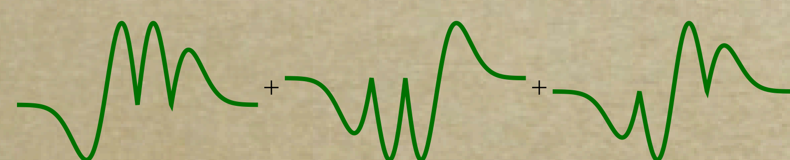


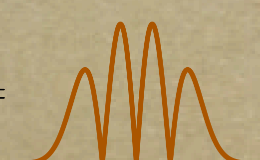
Example: N=3 majority particles

$$\psi_0(\mathbf{x}) = \mathcal{N}_N \left(\prod_{0 \le i < j \le N} x_{ij} \right) e^{-\sum_{k=0}^{N} x_k^2/2}$$

$\phi_0 =$ 

$\phi_1 =$ 

$\phi_2 =$ 

$\phi_3 =$ 

See also Deuretzbacher et al, PRL 2008

Few-body problem

For a single impurity problem and N majority fermions

N=2:

L. Guan et al PRL 2009

$$\phi_0 = \mathcal{N}_2 \; x_{12}x_{01}x_{02} \; e^{-\left(x_0^2+x_1^2+x_2^2\right)/2},$$
$$\phi_1 = \mathcal{N}_2 \; x_{12}\left(|x_{01}|x_{02} + x_{01}|x_{02}|\right) \; e^{-\left(x_0^2+x_1^2+x_2^2\right)/2},$$
$$\phi_2 = \mathcal{N}_2 \; x_{12}|x_{01}x_{02}| \; e^{-\left(x_0^2+x_1^2+x_2^2\right)/2}.$$

$$\psi_0 = \phi_0, \;\; \psi_1 = \sqrt{\frac{3}{8}}\phi_1, \;\; \psi_2 = \sqrt{\frac{1}{8}}(\phi_0 - 3\phi_2)$$

all fixed by spin and parity

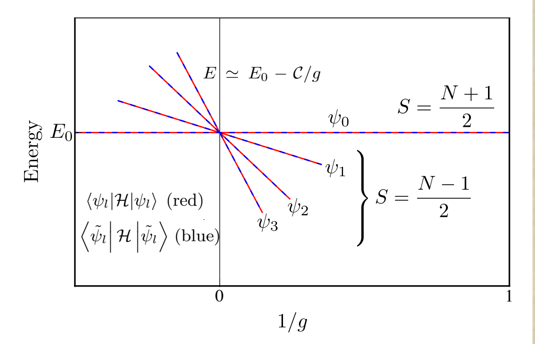
- Guan et al provided a solution for any N, but already for N=3 this did not match the result of recent numerics:

Gharashi, Blume PRL 2013

$$\tilde{\psi}_0 = \phi_0, \;\; \tilde{\psi}_1 = \sqrt{\frac{1}{5}}\phi_1, \;\; \tilde{\psi}_2 = \frac{1}{2}(\phi_0 - \phi_2), \;\; \tilde{\psi}_3 = \sqrt{\frac{1}{20}}(\phi_1 - 5\phi_3)$$

not all fixed by spin and parity

Strong-coupling ansatz



Inspired by the 3- and 4-body solutions we propose an ansatz:

For any N, the l'th wavefunction is a superposition of the basis functions with at most l absolute values

- Idea: cusps in the wavefunction reduce kinetic energy at finite repulsion — let us introduce these gradually
- Advantage: the problem is reduced to Gram-Schmidt orthogonalization

N=3:

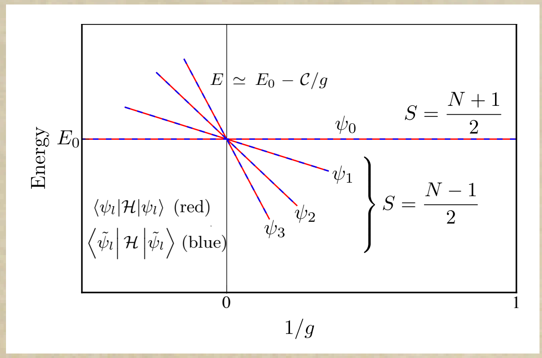
$$\tilde{\psi}_0 = \phi_0, \quad \tilde{\psi}_1 = \sqrt{\frac{1}{5}}\phi_1, \quad \tilde{\psi}_2 = \frac{1}{2}(\phi_0 - \phi_2), \quad \tilde{\psi}_3 = \sqrt{\frac{1}{20}}(\phi_1 - 5\phi_3)$$

$$\psi_0 = \phi_0, \qquad \psi_1 = \sqrt{\frac{1}{5}}(1.00188\phi_1 - 0.00941\phi_3), \qquad \psi_2 = \frac{1}{2}(\phi_0 - \phi_2), \qquad \psi_3 = \sqrt{\frac{1}{20}}(0.99246\phi_1 - 4.99996\phi_3)$$

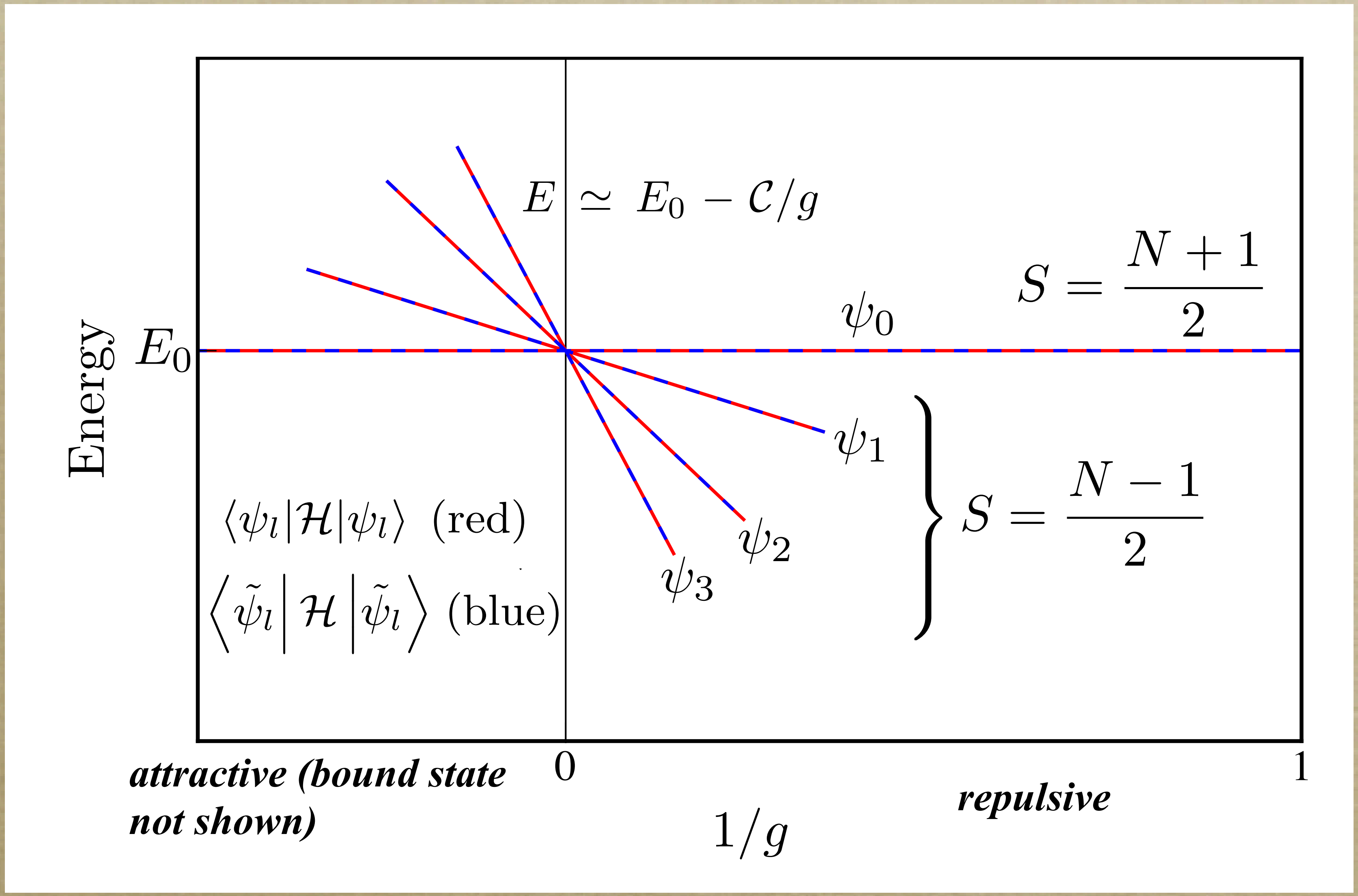
3-body: Guan et al PRL 2009
4-body: Gharashi, Blume PRL 2013

$|\langle \psi_l | \tilde{\psi}_l \rangle|$ *exceeds* 0.999993

4-body spectrum in TG limit



- For the four-body problem, our ansatz works very well



Perturbation theory in the TG limit

- We can also perform exact calculations in the TG limit, using the Hellmann-Feynman theorem

$$\mathcal{H} = \sum_{i=0}^{N} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right] + g \sum_{i<j} \delta(x_i - x_j)$$

$$\mathcal{C} = -\left.\frac{dE}{d(g^{-1})}\right|_{g\to\infty} = -\left.\left\langle \frac{\partial \mathcal{H}}{\partial (g^{-1})} \right\rangle\right|_{g\to\infty} \equiv \frac{\langle \Psi | \mathcal{H}' | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

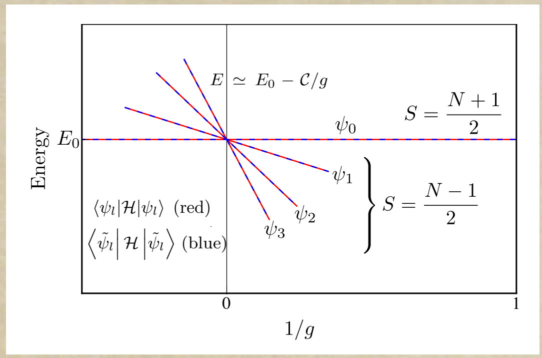
$$\begin{aligned} \mathcal{H}'_{ln} &= \langle \phi_l | \mathcal{H}' | \phi_n \rangle = \lim_{g\to\infty} g^2 \sum_{i=1}^{N} \int d\mathbf{x}\ \delta(x_{i0}) \phi_l \phi_n \\ &= \sum_{i=1}^{N} \int d\mathbf{x}\ \delta(x_{i0}) \left.\frac{\partial \phi_l}{\partial x_{i0}}\right|_{-}^{+} \left.\frac{\partial \phi_n}{\partial x_{i0}}\right|_{-}^{+}, \end{aligned}$$

This multidimensional integral cannot be calculated combinatorially

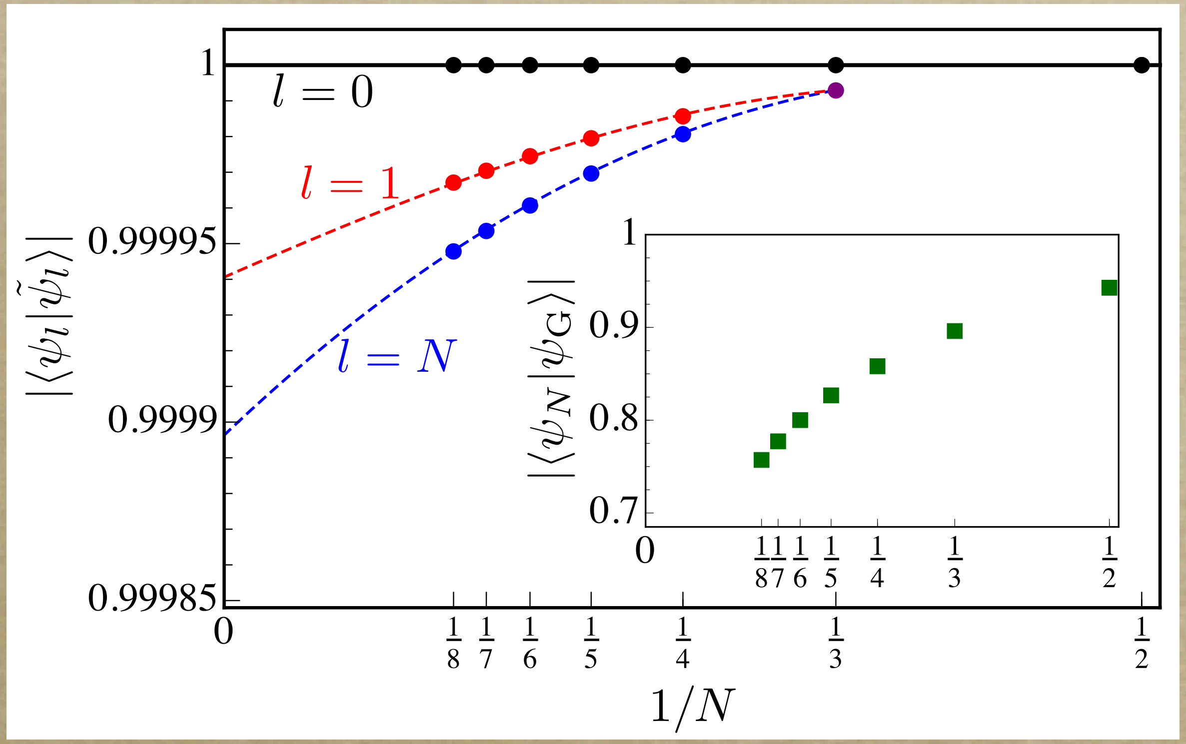
- *We are limited to N<10*

See also Volosniev et al, Nat Comm 2014

Comparison between exact solution and ansatz



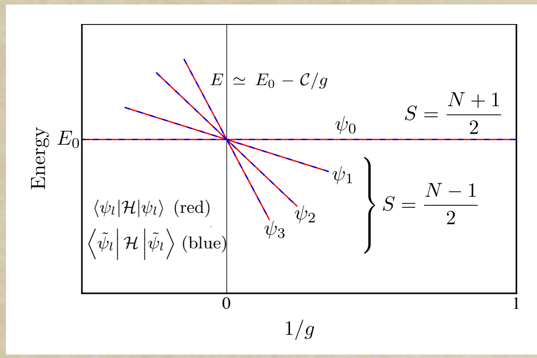
- Wavefunction overlap of exact and ansatz solutions exceed 0.9997 for all states up to *N*=8



Inset: Girardeau's ansatz, PRA 2010

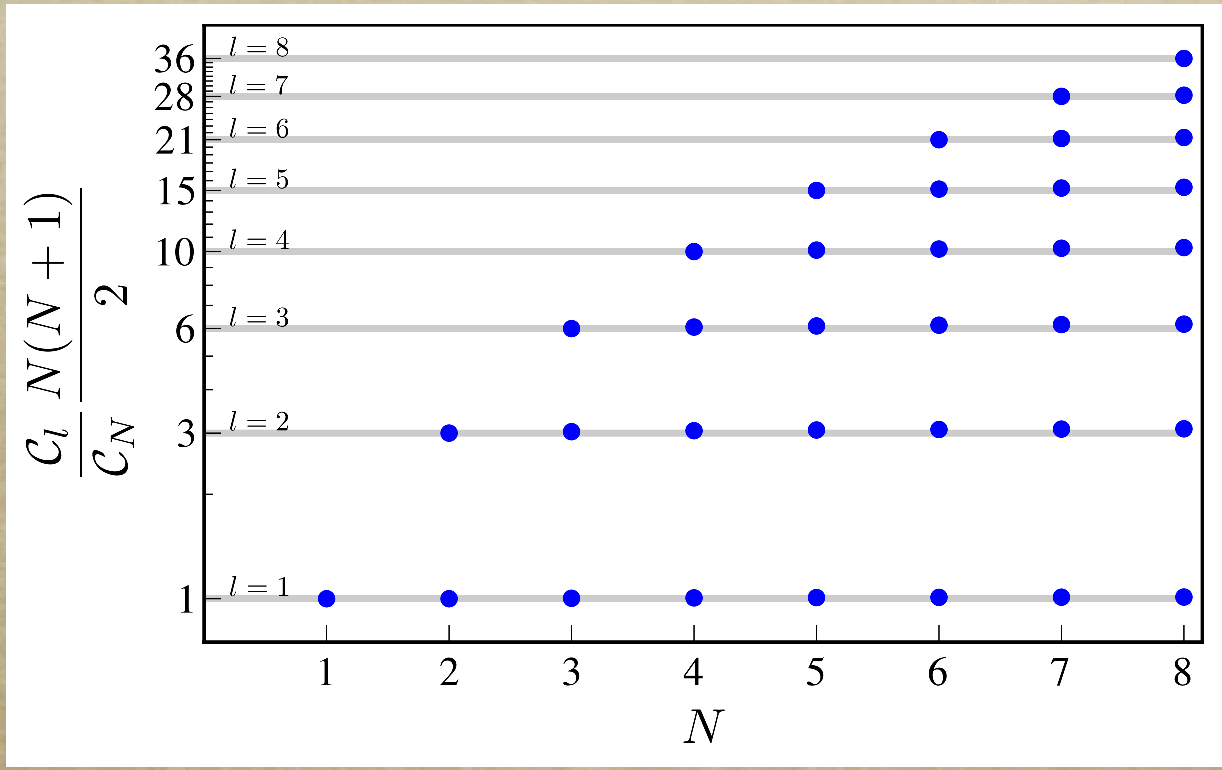
- Ground state wavefunction appears to extrapolate to an overlap ~ 0.9999

An approximate symmetry?



- We find an unexpected approximate relation (correct to within 3% for N up to 8):

$$\mathcal{C}_l \sim l(l+1)$$



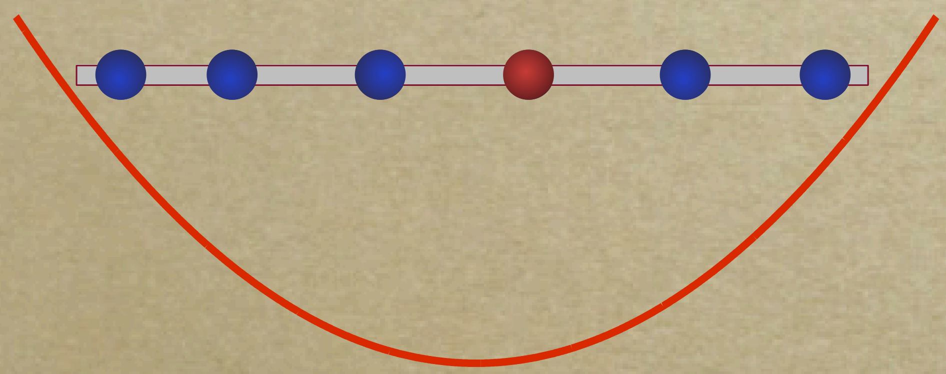
- This spectrum is intimately related to our ansatz

Harmonic Heisenberg model

- In the TG limit, we can write the Hamiltonian as a Heisenberg model:

$$\mathcal{H} \simeq E_0 - \frac{\mathcal{H}'}{g} = E_0 + \frac{\mathcal{C}_N}{g} \sum_{i=0}^{N-1} \left[J_i \mathbf{S}^i \cdot \mathbf{S}^{i+1} - \frac{1}{4} J_i \right]$$

Matveev PRL 2004
Volosniev et al, Nat Comm 2014
Deuretzbacher et al, PRA 2014



- Within our ansatz, using the approximate spectrum, we can calculate the nearest neighbour exchange constants

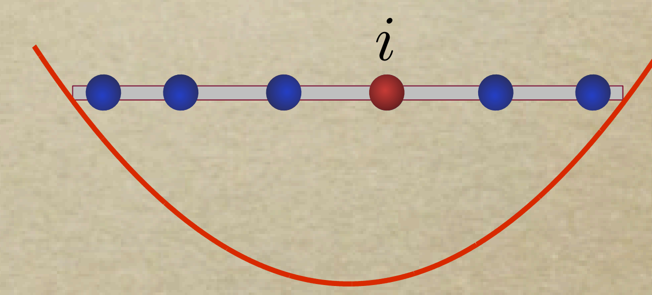
$$J_i = \frac{-\left(i - \frac{N-1}{2}\right)^2 + \frac{1}{4}(N+1)^2}{N(N+1)/2}$$

i is a particle index, not a site index

Wavefunctions in the ground state manifold

- We can solve the harmonic Heisenberg model exactly for the single impurity. The result is the family of discrete Chebyshev polynomials, known from approximation theory

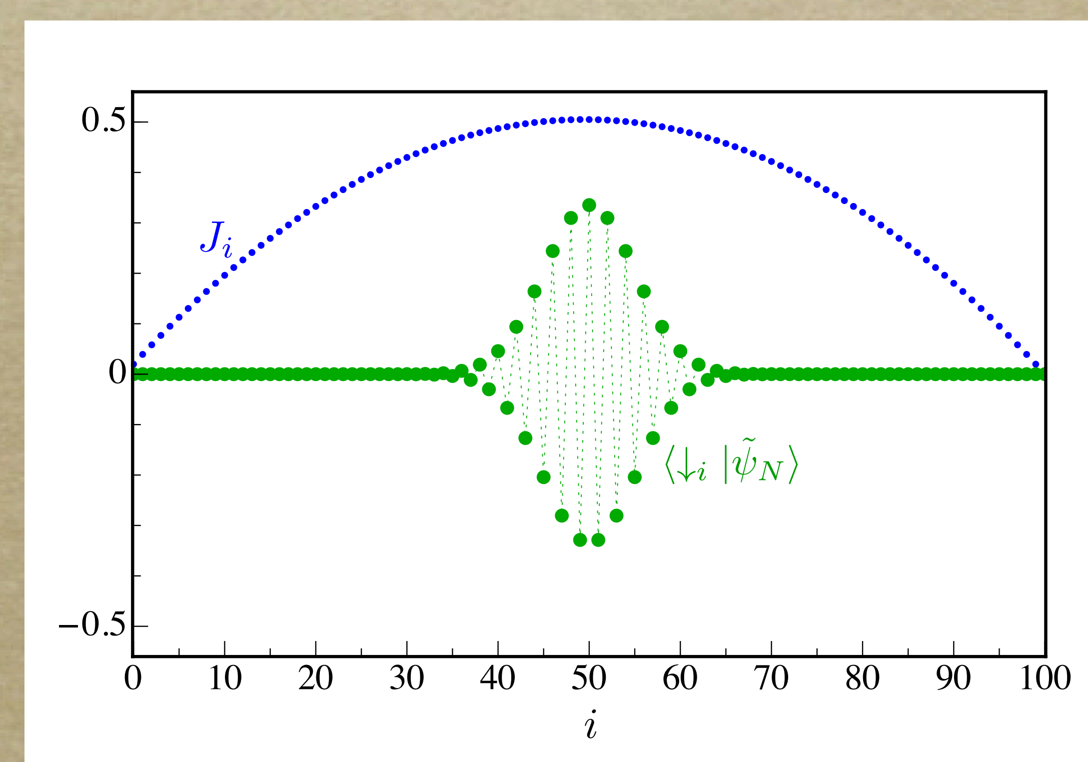
$$\left|\tilde{\psi}_l\right\rangle = \eta_l^{(N)} \sum_{i=0}^{N} \sum_{n=0}^{l} (-1)^n \binom{l+n}{n} \binom{N-n}{N-l} \binom{i}{n} \left|\downarrow_i\right\rangle$$



The ground state wavefunction is a sign-alternating Pascal's triangle

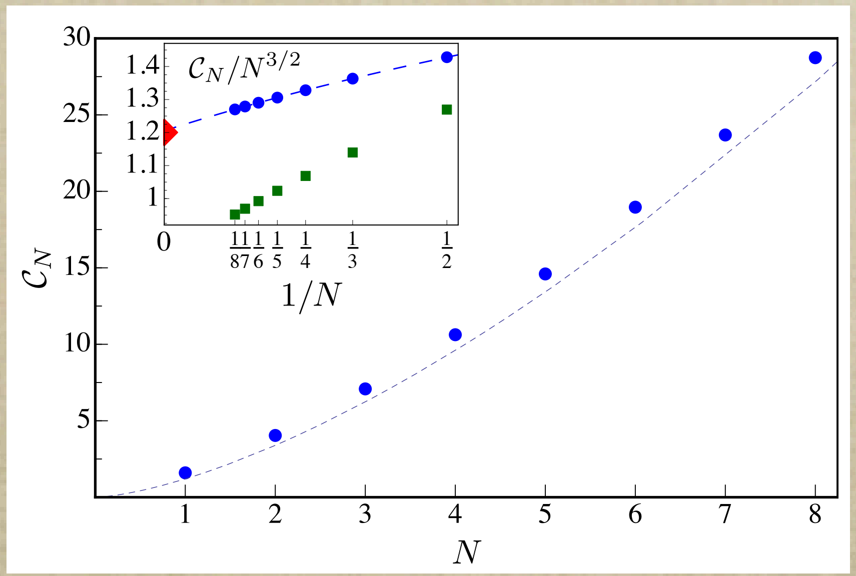
$$\left|\tilde{\psi}_N\right\rangle = \binom{2N}{N}^{-1/2} \sum_{i=0}^{N} (-1)^i \binom{N}{i} \left|\downarrow_i\right\rangle$$

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
1 5 10 10 5 1



Approaching the many-body limit

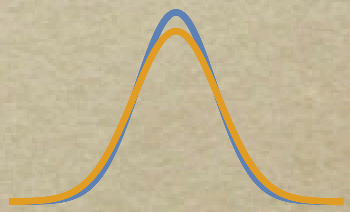
Contact of the ground state wavefunction



- *Approaches McGuire + LDA*

McGuire, J. Mat. Phys. 1965
Astrakharchik, Brouzos PRA 2013

Probability distribution of the impurity in the ground state wavefunction using LDA

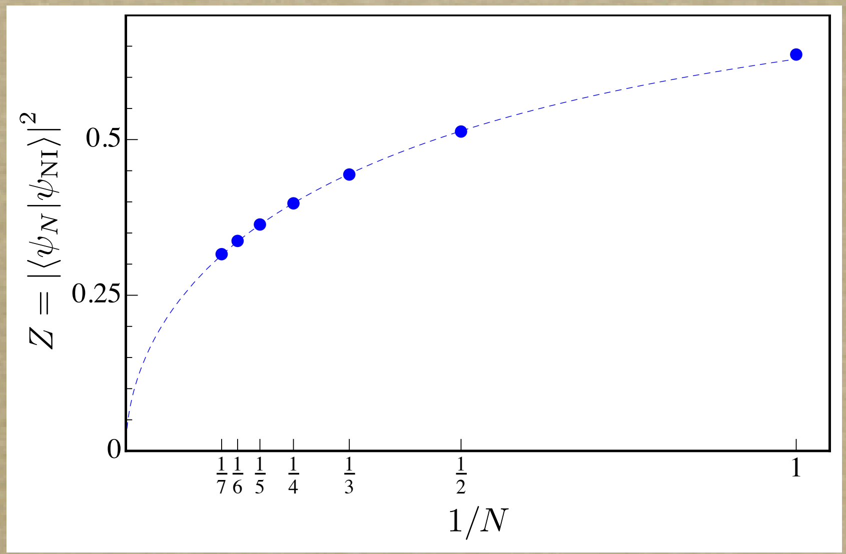


$$P_N(i) \simeq |\langle \downarrow_i | \tilde{\psi}_N \rangle|^2 = \binom{2N}{N}^{-1} \binom{N}{i}^2$$

$$P_N(x_0) \simeq \left(\frac{2}{\pi}\right)^{3/2} e^{-8x_0^2/\pi^2}$$

$$P_{\rm NI}(x_0) = e^{-x_0^2}/\sqrt{\pi}$$

Residue approaches zero as required by orthogonality catastrophe



Breathing modes

- Shift of energies in higher manifolds can be calculated using a dynamical SO(2,1) symmetry
    - *In the absence of a harmonic potential, the system is scale invariant in the TG limit*
    - *The introduction of the harmonic potential leads to an algebra with SO(2,1) commutation relations*

Pitaevskii and Rosch, PRA 1997

$$\delta E_1 = \left(1 + \frac{3}{4E_0}\right)\delta E_0$$

2D: Moroz PRA 2012

In the TG limit, the breathing modes form a tower of modes separated by twice the harmonic oscillator frequency. Away from TG limit this is $\delta E_1 - \delta E_0 = 3\delta E_0/4E_0$

Conclusions and outlook

- We proposed a *strong coupling ansatz* for a single impurity immersed in a 1D Fermi gas in a harmonic potential
  - Wavefunction overlaps with exact states exceed 0.9997 for all up to N=8
  - We obtained an approximate $l(l+1)$ spectrum
  - No small parameter — "weakly broken" symmetry?
- We obtained the model within which our approximation is exact
  - *Harmonic Heisenberg model - valid for any number of particles*
  - For the 2+2 problem, wavefunction overlap is $\gtrsim 0.99998$ when comparing with numerics
- The ground state manifold is formed from the discrete Chebyshev polynomials
- Mappings from fermions to bosons? SU(N) magnetism? Higher dimensions?

Acknowledgements

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Monash University

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Thank you!