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

Jesper Levinsen
Monash University, Melbourne

Collaboration with
Pietro Massignan (ICFO Barcelona)
Georg Bruun (Aarhus University)
Meera Parish (Monash University)

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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:

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

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

Wavefunctions in the Tonks-Girardeau limit:

\[ x_{01} e^{-(x_0^2 + x_1^2)/2} \]

|\[ x_{01} |e^{-(x_0^2 + x_1^2)/2} \]

Exact solution: Busch et al, Foundations of Physics 1998
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:**

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

- **Such wavefunctions all have the same kinetic energy and vanishing interaction energy**
Basis functions for an impurity in the TG limit

Example: N=3 majority particles

\[ \psi_0(x) = N_N \left( \prod_{0 \leq i < j \leq N} x_{ij} \right) e^{-\sum_{k=0}^{N} x_k^2/2} \]

\[ \phi_0 = \begin{array}{c}
\end{array} \]

\[ \phi_1 = \begin{array}{c}
\end{array} \]

\[ \phi_2 = \begin{array}{c}
\end{array} \]

\[ \phi_3 = \begin{array}{c}
\end{array} \]

See also Deuretzbacher et al, PRL 2008
For a single impurity problem and $N$ majority fermions

$N=2$:

$$
\begin{align*}
\phi_0 &= N_2 \, x_{12} x_{01} x_{02} \, e^{-(x_0^2 + x_1^2 + x_2^2)/2}, \\
\phi_1 &= N_2 \, x_{12} (|x_{01}|x_{02} + x_{01}|x_{02}|) \, e^{-(x_0^2 + x_1^2 + x_2^2)/2}, \\
\phi_2 &= N_2 \, x_{12}|x_{01}x_{02}| \, e^{-(x_0^2 + x_1^2 + x_2^2)/2}.
\end{align*}
$$

$$
\begin{align*}
\psi_0 &= \phi_0, & \psi_1 &= \sqrt{3} \, \phi_1, & \psi_2 &= \sqrt{\frac{1}{8}} (\phi_0 - 3\phi_2)
\end{align*}
$$

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:

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

not all fixed by spin and parity

L. Guan et al PRL 2009

Gharashi, Blume PRL 2013
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

$N=3$:

$$
\psi_0 = \phi_0, \quad \tilde{\psi}_1 = \sqrt{\frac{1}{5}} \phi_1, \quad \tilde{\psi}_2 = \frac{1}{2} (1 - \phi_1), \quad \tilde{\psi}_3 = \sqrt{\frac{1}{20}} (\phi_1 - 5\phi_3)
$$

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

$|\langle \psi_l | \tilde{\psi}_l \rangle|$ 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

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

\[
\mathcal{H}'_{ln} = \langle \phi_l | \mathcal{H}' | \phi_n \rangle = \lim_{g \to \infty} g^2 \sum_{i=1}^{N} \int dx \delta(x_i) \phi_l \phi_n
\]

\[
= \sum_{i=1}^{N} \int dx \delta(x_i) \frac{\partial \phi_l}{\partial x_i} \bigg|_+ \frac{\partial \phi_n}{\partial x_i} \bigg|_+
\]

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 \( N=8 \)

\[
|\langle \psi_l | \tilde{\psi}_l \rangle| \quad l = 0, 1, N
\]

Inset: Girardeau’s ansatz, PRA 2010

- Ground state wavefunction appears to extrapolate to an overlap \( \sim 0.9999 \)
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:

\[ H \approx E_0 - \frac{H'}{g} = E_0 + \frac{C_N}{g} \sum_{i=0}^{N-1} \left[ J_i S^i \cdot S^{i+1} - \frac{1}{4} J_i \right] \]

- 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

\[ |\tilde{{\psi}}_l\rangle = \eta_l^{(N)} \sum_{i=0}^{N} \sum_{n=0}^{l} (-1)^n \left( \begin{array}{c} l + n \\ n \end{array} \right) \left( \begin{array}{c} N - n \\ N - l \end{array} \right) \left( \begin{array}{c} i \\ n \end{array} \right) |\downarrow_i\rangle \]

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

\[ |\tilde{{\psi}}_N\rangle = \left( \begin{array}{c} 2N \\ N \end{array} \right)^{-1/2} \sum_{i=0}^{N} (-1)^i \left( \begin{array}{c} N \\ i \end{array} \right) |\downarrow_i\rangle \]
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

\[
P_N(i) \simeq |\langle \downarrow_i | \tilde{\psi}_N \rangle|^2 = \left( \frac{2N}{N} \right)^{-1} \left( \frac{N}{i} \right)^2 \quad P_N(x_0) \simeq \left( \frac{2}{\pi} \right)^{3/2} e^{-8x_0^2/\pi^2} \quad P_{NI}(x_0) = e^{-x_0^2}/\sqrt{\pi}
\]

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

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

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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