Exotic bound states and Bethe-ansatz solvability of a two-particle Hubbard model

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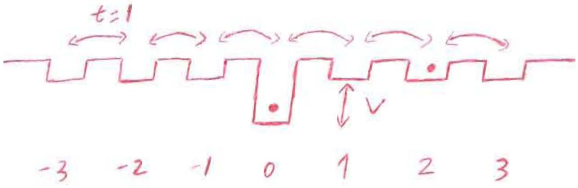
Outline

- A simple two-particle Bose-Hubbard model
  - similar to the negative Hydrogen ion H^- problem
  - a bound state in the continuum
  - protected by integrability
- Bethe-ansatz
  - only works for the odd-parity states!
  - half-integrable (in a loose sense)
- A Bethe-form checking algorithm
  - no diffraction in the odd-parity subspace
  - diffraction in the even-parity subspace
- A simple but nontrivial scattering problem

A lattice version of the H^- problem

The Hamiltonian (with only **two** particles):

$$\hat{H} = \sum_{x=-\infty}^{+\infty} \left[-(\hat{a}_x^\dagger \hat{a}_{x+1} + \hat{a}_{x+1}^\dagger \hat{a}_x) + \frac{U}{2} \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x \hat{a}_x \right] + V \hat{a}_0^\dagger \hat{a}_0.$$



The motivation:

- How many bound states?
- Interplay of U and V

Numerics first (No expectation of integrability)

How to filter a bound state out of the (majority) extended states?

- **The ultimate criterion**: a bound state, unlike an extended state, is insensitive to the boundary or boundary condition.

The algorithm:

- solve the eigenstates by exact-diagonalization on a lattice of size M_1
- for each eigenstate calculate the average of

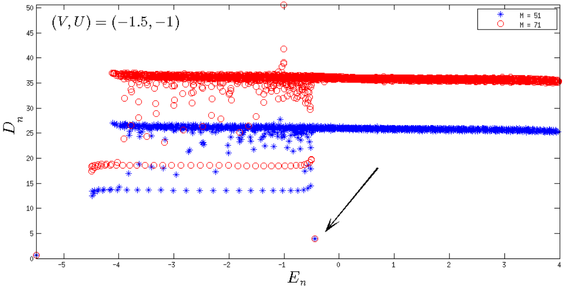
$$D = |x_1| + |x_2|$$

- a difference:

$$\begin{cases} D \to \text{const}, & \text{for a bound state,} \\ D \propto M_1, & \text{for an extended state.} \end{cases}$$

- repeat the procedure on a larger lattice with $M_2 > M_1$;
  Bound states $\Longleftrightarrow$ fixed D at fixed E

A weird bound state: embedded in the continuum!



An entity predicted by von Neumann & Wigner, Phys. Z. **30**, 465 (1929)

- admitted by theory:

$$E\psi = [-\nabla^2 + V(r)]\psi \quad \Longrightarrow \quad V(r) = E + \frac{\nabla^2\psi}{\psi}, \quad \parallel \psi \parallel = 1$$

- but *not* expected in real life!
- omitted in possibly every textbook on quantum mechanics

Hidden integrability!

Bound-state-in-the-continuum is a *non-generic* object

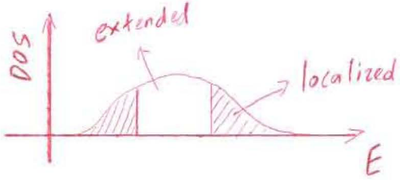
Degeneracy between a localized state ψ_b and an extended state ψ_e is *unstable*.

$$H_{subspace} = \begin{pmatrix} E & \delta \\ \delta & E \end{pmatrix}, \quad \delta \to 0.$$

New eigenstates:

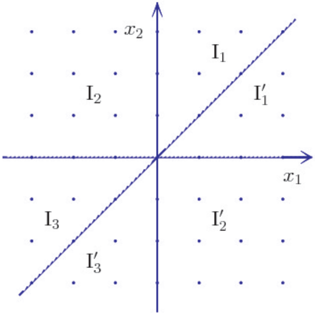
$$\psi_\pm = \frac{1}{\sqrt{2}}(\psi_b \pm \psi_e).$$

Both are now extended!



Mott's sharp mobility edges in a disordered lattice!

Bethe Ansatz



Configuration space

- two particles in 1D = one particle in 2D
- infinite lattice assumed

In region I_1:

$$
\begin{aligned}
f = {} & A_1 e^{+ik_1x_1+ik_2x_2} + A_2 e^{+ik_1x_1-ik_2x_2} \\
& + A_3 e^{-ik_1x_1+ik_2x_2} + A_4 e^{-ik_1x_1-ik_2x_2} \\
& + A_5 e^{+ik_2x_1+ik_1x_2} + A_6 e^{-ik_2x_1+ik_1x_2} \\
& + A_7 e^{+ik_2x_1-ik_1x_2} + A_8 e^{-ik_2x_1-ik_1x_2}
\end{aligned}
$$

In regions I_2 and I_3, A's replaced by B's and C's.

Away from the interfaces:

$$Hf = Ef, \quad E = -2(\cos k_1 + \cos k_2),$$

already satisfied.

Linking the wave functions on the interfaces

A set of 24 linear equations about the 24 unknowns A's, B's, C's.

- parametrized by k_1 and k_2
- homogeneous

Depending on the **parity** $(x_i \leftrightarrow -x_i)$:

- Even-parity,
$$f(x_1, x_2) = +f(-x_1, -x_2),$$
not self-consistent! Ansatz wrong!
- Odd-parity,
$$f(x_1, x_2) = -f(-x_1, -x_2),$$
self-consistent!

A subtle fact missed by J. B. McGuire!

J. B. McGuire, "*Study of exactly soluble one-dimensional N-body problems*", J. Math. Phys. 5, 622 (1964).

Two odd-parity bound states

Suppose $V < 0$ (The $V > 0$ case is similar):

- If $2V < U < V$, there exists an odd-parity bound state

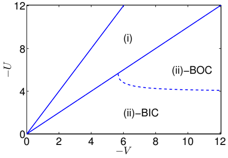
$$E_b = -\sqrt{V^2 + 4} - \sqrt{(V - U)^2 + 4}.$$

  Not a bound state in the continuum (BIC).

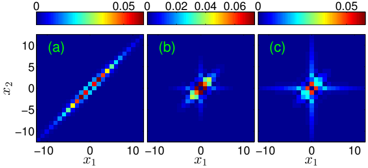
- If $V < U < 0$, there exists an odd-parity bound state

$$E_b = -\sqrt{V^2 + 4} + \sqrt{(V - U)^2 + 4}.$$

  It can be a bound state in the $[-4, +4]$ continuum!
  For example, if $(V, U) = (-2, -0.5)$, then $E_b = -0.3284$.



Phase diagram



Profiles of the BICs

The problem of the boundary and completeness

From an infinite lattice to a finite lattice:

- Now the boundary condition is not so easy to handle
- Bethe equations (for k_1 and k_2) very complicated!
  - no idea how to solve them
  - no idea how to exhaust the solutions
- Are the odd-parity states **still** in the Bethe-form?
- Are **all** the odd-parity states in the Bethe-form?

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Analytically difficult — so do it numerically:

Given a wave function, how to check that it is in the Bethe-form or not?
Or, given an array, is it a superposition of (finite) exponentials?

$$\begin{matrix} 2 & 2 & 3 & 4 & 6 & 19 \\ 1 & 1 & 2 & 3 & 5 & 2 \\ 2 & 2 & 3 & 4 & 6 & 1 \\ 4 & 4 & 5 & 6 & 8 & 8 \\ 8 & 8 & 9 & 10 & 12 & 0 \\ 0 & 3 & 5 & 2 & 9 & 1 \end{matrix}$$

A Bethe-form checking algorithm

An example: Is this array a superposition of **two** exponentials?

$$\{F_n\} = 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, \ldots$$

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$$\{F_n\} = 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, \ldots$$

Yes, it is! Because it is the Fibonacci array:

$$F_{n+2} = F_{n+1} + F_n,$$

and **linear recursive relation implies sum of exponentials**! In the transfer-matrix formalism,

$$\begin{pmatrix} F_{n+2} \\ F_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix}.$$

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Actually, De Moivre's formula:

$$F_n = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^n - \left(\frac{1-\sqrt{5}}{2} \right)^n \right].$$

The reverse is also true

Suppose ($c_i \neq c_j$ if $i \neq j$)

$$G_n = w_1 e^{c_1 n} + w_2 e^{c_2 n} + w_3 e^{c_3 n} + w_4 e^{c_4 n}, \quad n \in \mathcal{N}$$

then

$$G_{n+4} = r_3 G_{n+3} + r_2 G_{n+2} + r_1 G_{n+1} + r_0 G_n,$$

regardless of the values of the w's.

The r's are determined by

$$\begin{pmatrix} 1 & e^{c_1} & e^{2c_1} & e^{3c_1} \\ 1 & e^{c_2} & e^{2c_2} & e^{3c_2} \\ 1 & e^{c_3} & e^{2c_3} & e^{3c_3} \\ 1 & e^{c_4} & e^{2c_4} & e^{3c_4} \end{pmatrix} \begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix} = \begin{pmatrix} e^{4c_1} \\ e^{4c_2} \\ e^{4c_3} \\ e^{4c_4} \end{pmatrix}$$

Then check it!

Take a slice of f, $x_1 = $ const,

$$g_{x_2} \equiv f(x_1, x_2) = w_1 e^{ik_1 x_2} + w_2 e^{-ik_1 x_2} + w_3 e^{ik_2 x_2} + w_4 e^{-ik_2 x_2}.$$

Consider the linear equation

$$\begin{pmatrix} g_n & g_{n+1} & g_{n+2} & g_{n+3} \\ g_{n+1} & g_{n+2} & g_{n+3} & g_{n+4} \\ g_{n+2} & g_{n+3} & g_{n+4} & g_{n+5} \\ g_{n+3} & g_{n+4} & g_{n+5} & g_{n+6} \end{pmatrix} \begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix} = \begin{pmatrix} g_{n+4} \\ g_{n+5} \\ g_{n+6} \\ g_{n+7} \end{pmatrix}.$$

- A **necessary** condition: r's **independent** of n!

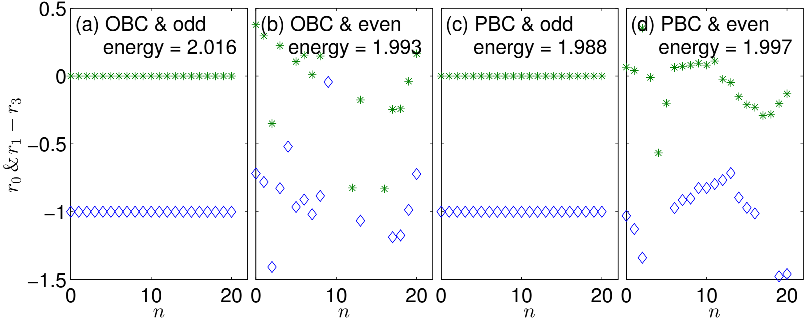
$$\begin{aligned} r_0 &= -1, \\ r_1 &= e^{ik_1} + e^{-ik_1} + e^{ik_2} + e^{-ik_2} = -E(k_1, k_2), \\ r_2 &= -(e^{ik_1} + e^{-ik_1})(e^{ik_2} + e^{-ik_2}) - 2, \\ r_3 &= r_1. \end{aligned}$$

- The exponents can be determined from the values of the r's

$$g_{n+4} = r_0 g_n + r_1 g_{n+1} + r_2 g_{n+2} + r_3 g_{n+3}$$

Odd vs. Even

An example: a 111-site lattice and $(V, U) = (-2, -2)$,

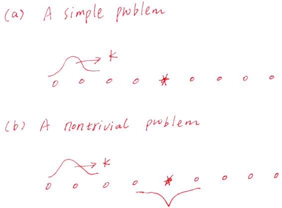


For both open and periodic boundary conditions,

- All odd-parity states are in the Bethe-form!
- All even-parity states are not in the Bethe-form!

Summary

- A half-integrable model
  - All odd-parity states are in the Bethe-form
  - All even-parity states are NOT in the Bethe-form
- A layman's algorithm for Bethe-form checking
- Exotic bound states
  - Bound states in the continuum
  - Bound states at the threshold
- How about dynamics? A scattering problem:



D. Braak, JMZ, and M. Kollar, arXiv:1403.6875; JMZ, D. Braak, and M. Kollar, PRA **87**, 023613 (2013); JMZ, D. Braak, and M. Kollar, PRL **109**, 116405 (2012)