Hubbard model: Bethe anzatz and the Lieb-Wu equations made easy

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Two-site Hubbard model, one electron $\uparrow$ and one electron $\downarrow$, 4 states

$$|\uparrow\downarrow, 0\rangle |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |0, \uparrow\downarrow\rangle$$

Hamiltonian matrix:

$$\begin{pmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & 0-t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{pmatrix}$$

Characteristic polynomial:

Det(E-H)=0 $\Rightarrow E(E-U)(E^2 - EU - 4t^2)$

- One triplet state:

$$E = 0 \;\; \text{with} \;\; |\Psi\rangle \sim |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle$$

- Three singlet states:

$$E = U \quad \text{with} \;\; |\Psi\rangle \sim |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle$$

$$E_{\pm} = \frac{U \pm \sqrt{U^2 + 16t^2}}{2}$$

• Bethe ansatz (1931) : Solution by Bethe of the quantum Heisenberg antiferromagnetic chain for any number of spins
• Lieb and Wu (1968) : Solution by Bethe ansatz of the 1D-Hubbard chain **for any number of sites and electrons**

Lieb and Wu equations for the 1D-model for 2 sites:

A) **Two-electron case, two sites** (one electron $\uparrow$, one electron$\downarrow$)

$$E = -t \cos k_1 - t \cos k_2$$

with k_1, k_2 solutions of the Lieb-Wu equations (here, with L sites)

- Triplet state

$$e^{ik_1 L} = e^{ik_2 L} = 1$$

- Singlet states

$$e^{ik_1 L} = \frac{\sin k_1 - \sin k_2 + \frac{iU}{t}}{\sin k_1 - \sin k_2 - \frac{iU}{t}}$$
$$e^{ik_2 L} = \frac{\sin k_2 - \sin k_1 + \frac{iU}{t}}{\sin k_2 - \sin k_1 - \frac{iU}{t}}$$

Rewriting of the equations, denoting $X = \sin k_1 - \sin k_2$

$$e^{ik_1 L} = \frac{X + \frac{iU}{t}}{X - \frac{iU}{t}} = -e^{-ik_2 L}$$

which gives the first equation:

$$e^{i(k_1+k_2)L} = 1 and \ \cos k_1 L = \frac{X^2 - \frac{U^2}{t^2}}{X^2 + \frac{U^2}{t^2}}$$
$$\sin k_1 L = \frac{\frac{2XU}{t}}{X^2 + \frac{U^2}{t^2}}$$
$$\sin k_1 L = 2 \sin \frac{k_1 L}{2} \cos \frac{k_1 L}{2}$$
$$\cos k_1 L = 2 \cos^2 \frac{k_1 L}{2} - 1$$

Then after some manipulation

$$\tan \frac{k_1 L}{2} = \frac{U}{t(\sin k_1 - \sin k_2)}$$

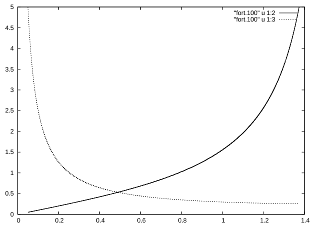
In the case of two sites, $L = 2$ and $k_1 + k_2 = 0$

$$\tan k_1 = \frac{U}{2t \sin k_1}$$

With $E = -2t \cos k_1$ we recover the result of the direct diagonalization:

$$E^2 - UE - 4t^2 = 0$$

Graphical way of looking at the solution.



There is one solution $|E| > 2t$ so the representation $E = -2t\cos k_1$ does not seem to work...**What does happen?**

In fact, we have to solve the equation **in the complex plane!** Let us write $k = x + iy$
The energy writes

$$E = -2t\cos k = -t(e^{ik} + e^{-ik}) = -t[\cos x(e^{-y} + e^{y}) + i\sin x(e^{-y} - e^{y})]$$

The imaginary part must be zero, so $\sin x = 0$ since we exclude the real axis ($y = 0$).
The missing solution so that $|E| > 2t$ must correspond to $x = \pi$

$$E = t(e^{-y} + e^{y})$$

and

$$y = cosh^{-1}(\frac{2E}{t})$$

On the other hand

$$\tan k = \frac{\sin k}{\cos k} = \frac{U}{2t \sin k}$$

$$\frac{e^{ik} - e^{-ik}}{i(e^{ik} + e^{-ik})} = \frac{iU}{2t(e^{ik} - e^{-ik})}$$

$$2t(e^{ik} - e^{-ik})^2 = -U(e^{ik} + e^{-ik})$$

$$2t(e^{2ik} + e^{-2ik} - 2) = -U(e^{ik} + e^{-ik})$$

Let us write $k = \pi + iy$ and write the real and imaginary part

$$t\left[(e^{-2y} + e^{2y}) - 2\right] = -U \cos x(e^{-y} + e^{y}))$$

$$-1 = -\frac{U(e^{-y} - e^{y})}{t(e^{-2y} - e^{2y})}$$

which with $E = t(e^{-y} + e^{y})$ gives

$$E = \frac{U \pm \sqrt{U^2 + 16t^2}}{2}$$

The solution E must be positive so we recover the missing solution and the complex k given by

$$k = (\pi, \cosh^{-1}\left[\frac{U}{t} + \sqrt{(\frac{U}{t})^2 + 16}\right])$$

B) **General Lieb-Wu equations** (N= Total number of electrons, M = number of electrons $\downarrow$, L= number of sites)

$$e^{ik_jL} = \prod_{l=1}^{M} \frac{\lambda_l - \sin k_j - \frac{iU}{2t}}{\lambda_l - \sin k_j + \frac{iU}{2t}} \quad j = 1, \ldots, N$$

and

$$\prod_{l=1}^{M} \frac{\lambda_l - \sin k_j - \frac{iU}{2t}}{\lambda_l - \sin k_j + \frac{iU}{2t}} = \prod_{m=1\ m\neq l}^{M} \frac{\lambda_l - \lambda_m - \frac{iU}{t}}{\lambda_l - \lambda_m + \frac{iU}{2t}} \quad l = 1, \ldots, M$$

with

$$E = -t \sum_{i=1}^{N} \cos k_i + \frac{U}{2t}(L - 2N)$$

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