Report 1

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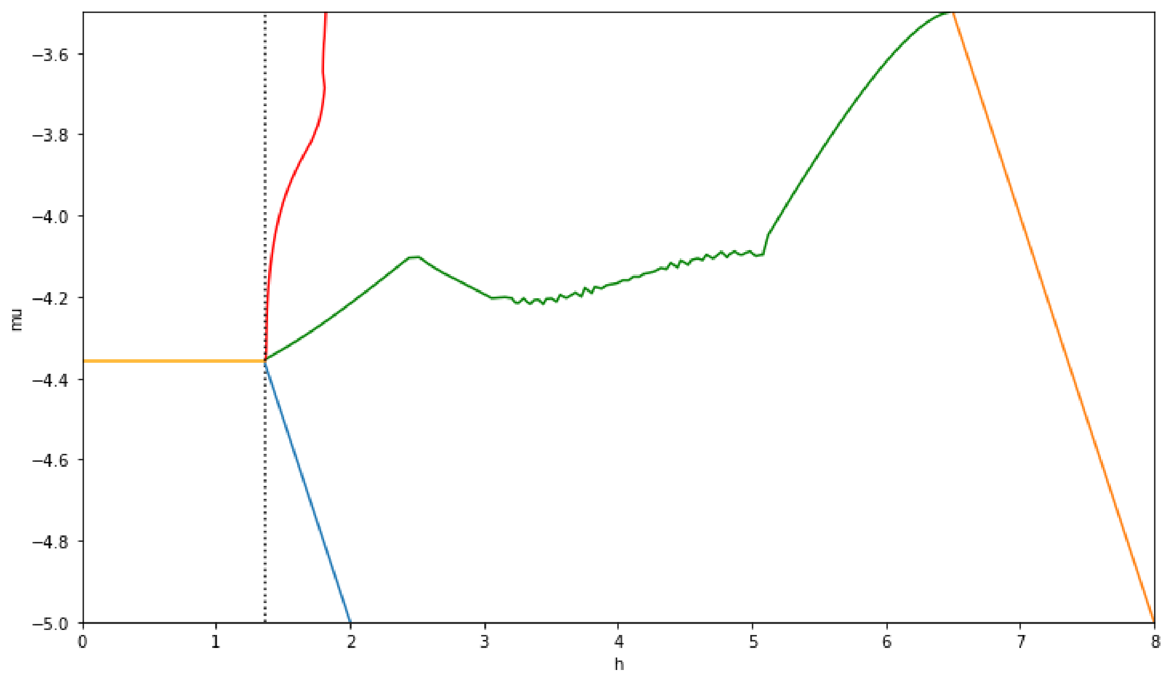
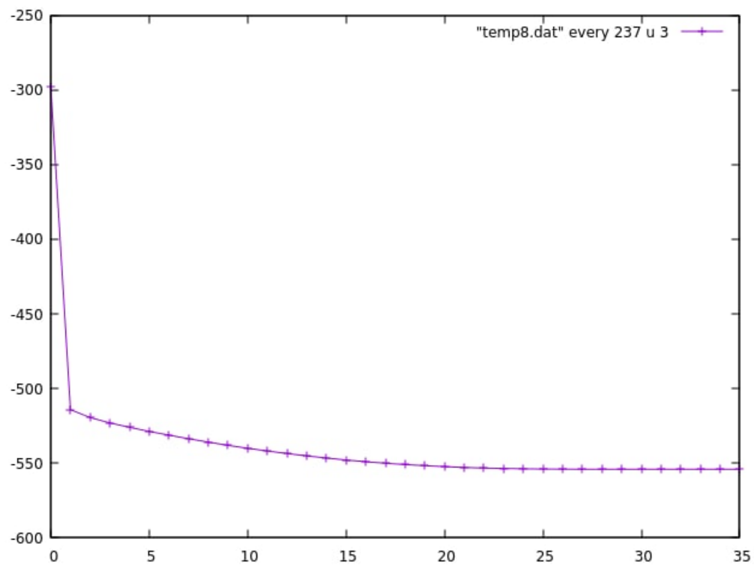
I've numerically studied the phase diagram of $L * W$ repulsive Hubbard ladder of length $L = 60$ with number of legs $W = 2$ on $\mu - h$ plane. This case requires more computational resources than that of $L = 40$. μ and h values were approximated using finite differences instead of derivatives. The diagram looks as follows:

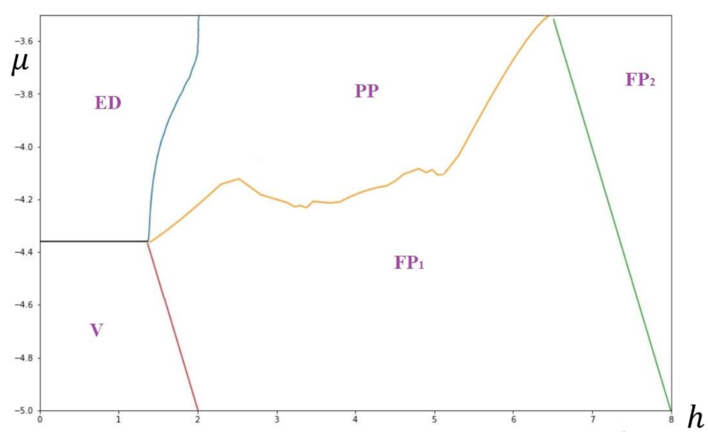


The diagram was calculated for all possible values of $E(N_1, N_2)$ where $N_1, N_2 = 1...120$. All the necessary E points were calculated using $DMRG$ method as implemented in $ALPS$ Python package. All points have the truncation error $< 10^{-7}$. Convergence of the algorithm could be controlled via NUMBER OF SWEEPS and MAXSTATES parameters, that were 1800 and 18 for most of the points. For the points with truncation error of $10^{-7} - 10^{-8}$ another check for convergence was conducted using mps_optim-impementation of DMRG.

Here's the graph of Energy convergence vs number of sweeps for $Nup = 73$ and $Ndown = 71$ obtained using *mps_optim* procedure with 35 sweeps and 1800 maxstates. Results for the ground-state energy is equivalent to the one of standard DMRG up to the third sign.

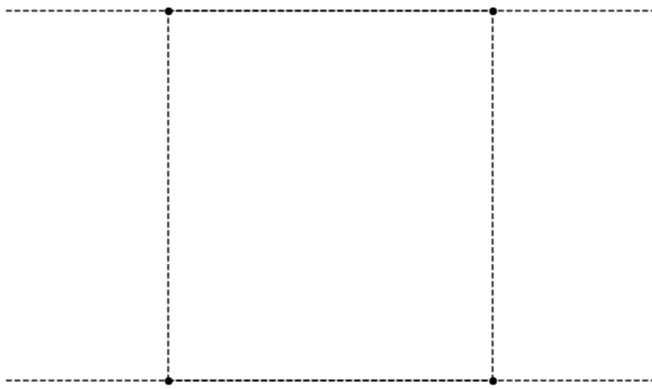


Firstly, the diagram looks just the same as the one for $L = 40$ and number of legs $W = 2$.



As one can easily see, the boundary between ED and PP phases has different position from that of $1D$-chain.

Also hamiltonians of ladders with 1..4 legs for $N = 1$ (which is equivalent to $U = 0$) were diagonalized using standard procedure. The two-leg ladder looks as two 1D chains connected to each other on every n:



Single-particle hamiltonian of a two-leg ladder is:

$$\hat{H} = \sum_{i,j=1,2} -t(a^{\dagger}_{i,j} a_{1+1,j} + h.c.) - t_{\perp}(a^{\dagger}_{i,1} a_{i,2} + h.c.) \tag{1}$$

To diagonalize it one should first switch to momentum-representation using Fourier-transformation and then find eigenvalues and eigenvectors of the obtained hamiltonian. Fourier-transformed creation-annihilation operators look as follows:

$$a_i = \frac{1}{\sqrt{L}} \sum_{l} a_k e^{ikx_i} \tag{2}$$

$$a^{\dagger}_i = \frac{1}{\sqrt{L}} \sum_{l} a^{\dagger}_k e^{-ikx_i} \tag{3}$$

Plugging (2) and (3) into $\hat{H}$ we obtain:

$$\hat{H} = \hat{H}_{\parallel,1leg} + \hat{H}_{\parallel,2leg} + \hat{H}_{\perp} \tag{4}$$

$$\hat{H}_{\parallel,1leg} = -\frac{t}{L} \sum_{i} (a^{\dagger}_k a_q e^{iqx_{i+1} - ikx_i} + a^{\dagger}_q a_k e^{iqx_{i+1} - ikx_i}) = -\frac{t}{L} \sum_{i} (a^{\dagger}_k a_q e^{i(q-k)x_i} e^{iqa} + a^{\dagger}_q a_k e^{i(k-q)x_i} e^{-iqa}) \tag{5}$$

Here one can see the delta function of the form:

$$\delta_{k,q}(x_i) = \delta_{q,k}(x_i) = \frac{1}{L} \sum_{i} e^{i(q-k)x_i} = \frac{1}{L} \sum_{i} e^{i(k-q)x_i} \tag{6}$$

Then $\hat{H}_{\parallel,1leg}$ takes the form:

$$\hat{H}_{\parallel,1leg} = \sum_{i} -t(\sum_{i} -t(a^{\dagger}_k a_k e^{ika} + a^{\dagger}_k a_k e^{-ika}) \tag{7}$$

That leads us to standard free 1D energy   cosine, but as energy is defined up to the arbitrary constant we'll take the constant equal to 1:

$$\hat{H}_{\parallel,1leg} = \sum_i (1 - 2tcos(ka))a^\dagger_{k,1}a_{k,1} = \sum_i \epsilon_k a^\dagger_{k,1}a_{k,1} \tag{8}$$

Diagonalization of $\hat{H}_{\parallel,2leg}$ leads us to the same relation:

$$\hat{H}_{\parallel,2leg} = \sum_i (1 - 2tcos(ka))a^\dagger_{k,2}a_{k,2} = \sum_i \epsilon_k a^\dagger_{k,2}a_{k,2} \tag{9}$$

Now to the most interesting part:

$$\hat{H}_\perp = -t_\perp \sum_i (a^\dagger_{i,1}a_{i,2} + a^\dagger_{i,2}a_{i,1}) \tag{10}$$

$$\hat{H}_\perp = -\frac{t_\perp}{L} \sum_{k,q} (a^\dagger_{k,1}a_{q,2}e^{i(k-q)x_i} + a^\dagger_{q,2}a_{k,1}e^{i(q-k)x_i}) \tag{11}$$

$$\hat{H}_\perp = -t_\perp \sum_k (a^\dagger_{k,1}a_{k,2} + a^\dagger_{k,2}a_{k,1}) \tag{12}$$

Finally our hamiltonian takes the form:

$$\hat{H} = \sum_k \epsilon_k a^\dagger_{k,1}a_{k,1} + \sum_k \epsilon_k a^\dagger_{k,2}a_{k,2} - t_\perp \sum_k (a^\dagger_{k,1}a_{k,2} + a^\dagger_{k,2}a_{k,1}) \tag{13}$$

Let's rewrite the hamiltonian in matrix form to make it easier to diagonalize:

$$\begin{pmatrix} a^\dagger_{k,1} & a^\dagger_{k,2} \end{pmatrix} \begin{pmatrix} \epsilon_k & -t_\perp \\ -t_\perp & \epsilon_k \end{pmatrix} \begin{pmatrix} a_{k,1} \\ a_{k,2} \end{pmatrix} = \begin{pmatrix} c^\dagger_{k,1} & c^\dagger_{k,2} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} c_{k,1} \\ c_{k,2} \end{pmatrix} \tag{14}$$

To find eigenvalues one has to solve the equation:

$$\begin{vmatrix} \epsilon_k - \lambda & -t_\perp \\ -t_\perp & \epsilon_k - \lambda \end{vmatrix} = 0 \tag{15}$$

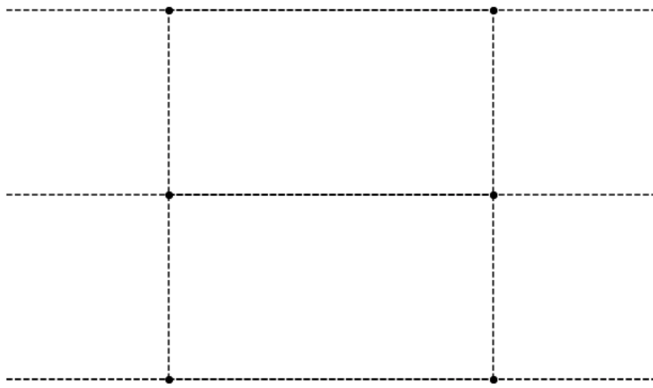
$$(\epsilon_k - \lambda)^2 - (t_\perp)^2 = 0 \tag{16}$$

$$\lambda_{1,2} = \epsilon_k \pm t_\perp \tag{17}$$

Then the diagonalized hamiltonian takes the form:

$$\hat{H} = \sum_k (\epsilon_k - t_\perp)c^\dagger_{k,1}c_{k,1} + \sum_k (\epsilon_k + t_\perp)c^\dagger_{k,2}c_{k,2} \tag{18}$$

3-leg ladder has the same structure as before, but there are 3 1D-chains now:



For a 3-leg ladder the approach is just the same:

$$\hat{H} = -t\sum_i a^{\dagger}_{i,1}a_{i+1,1} + h.c. - t\sum_i a^{\dagger}_{i,2}a_{i+1,2} + h.c. - t\sum_i a^{\dagger}_{i,3}a_{i+1,3} + h.c. -$$
$$-t_+\sum_i (a^{\dagger}_{i,1}a_{i,2} + a^{\dagger}_{i,2}a_{i,1}) - t_\perp\sum_i (a^{\dagger}_{i,2}a_{i,3} + a^{\dagger}_{i,3}a_{i,2})$$

We obtain the same $\epsilon_k = (1 - 2tcos(ka))$ along the leg and the hamiltonian then takes the form:

$$\hat{H} = \sum_k \epsilon_k a^{\dagger}_{k,1}a_{k,1} + \sum_k \epsilon_k a^{\dagger}_{k,2}a_{k,2} + \sum_k \epsilon_k a^{\dagger}_{k,3}a_{k,3} - t_\perp(\sum_k a_{k,1}{}^{\dagger}a_{k,2} + a_{k,2}{}^{\dagger}a_{k,1} + a_{k,2}{}^{\dagger}a_{k,3} + a_{k,3}{}^{\dagger}a_{k,2})$$

$$\begin{pmatrix} a^{\dagger}_{k,1} & a^{\dagger}_{k,2} & a^{\dagger}_{k,3} \end{pmatrix} \begin{pmatrix} \epsilon_k & -t_\perp & 0 \\ -t_+ & \epsilon_k & -t_\perp \\ 0 & -t_\perp & \epsilon_k \end{pmatrix} \begin{pmatrix} a_{k,1} \\ a_{k,2} \\ a_{k,3} \end{pmatrix} = \begin{pmatrix} c^{\dagger}_{k,1} & c^{\dagger}_{k,2} & c^{\dagger}_{k,3} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \begin{pmatrix} c_{k,1} \\ c_{k,2} \\ c_{k,3} \end{pmatrix}$$

$$\begin{vmatrix} \epsilon_k - \lambda & -t_\perp & 0 \\ -t_\perp & \epsilon_k - \lambda & -t_\perp \\ 0 & -t_\perp & \epsilon_k - \lambda \end{vmatrix} = 0 \tag{19}$$

Expanding along the first row we obtain:

$$(\epsilon_k - \lambda)((\epsilon_k - \lambda)^2 - t_\perp{}^2) + t_\perp(-t_\perp(\epsilon_k - \lambda)) = 0 \tag{20}$$

Taking the common factor out of the brackets:

$$(\epsilon_k - \lambda)((\epsilon_k - \lambda)^2 - 2t_\perp{}^2) = 0 \tag{21}$$

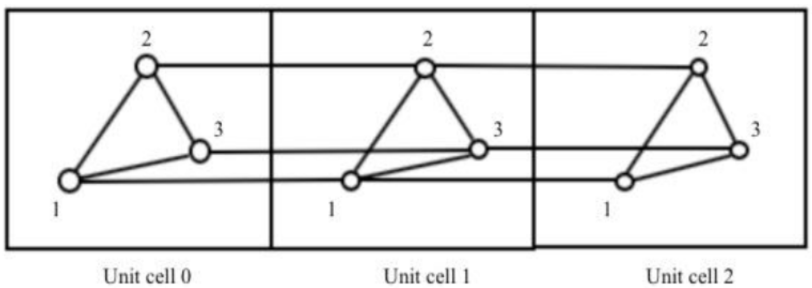
Lambdas then are:

$$\begin{aligned}\lambda_1 &= \epsilon_k \\ \lambda_2 &= \epsilon_k + t_\perp\sqrt{2} \\ \lambda_3 &= \epsilon_k - t_\perp\sqrt{2}\end{aligned} \tag{22}$$

So diagonalized hamiltonian will be:

$$\hat{H} = \sum_k \epsilon_k c^\dagger_{k,1} c_{k,1} + \sum_k (\epsilon_k - t_\perp\sqrt{2}) c^\dagger_{k,1} c_{k,1} + \sum_k (\epsilon_k + t_\perp\sqrt{2}) c^\dagger_{k,2} c_{k,2} \tag{23}$$

Next configuration is so-called toblerone-shaped 3-leg ladder. It is the same as standard 3leg ladder, but it has cylindrical boundary conditions along y-axis.



Technically speaking, toblerone-shaped lattice has one extra hopping term from the 3rd leg to the 1st:

$$\begin{aligned}\hat{H} = \sum_k \epsilon_k a^\dagger_{k,1} a_{k,1} + \sum_k \epsilon_k a^\dagger_{k,2} a_{k,2} + \sum_k \epsilon_k a^\dagger_{k,3} a_{k,3} - \\ -t_\perp(\sum_k a_{k,1}{}^\dagger a_{k,2} + a_{k,2}{}^\dagger a_{k,1} + a_{k,2}{}^\dagger a_{k,3} + a_{k,3}{}^\dagger a_{k,2} + a_{k,3}{}^\dagger a_{k,1} + a_{k,1}{}^\dagger a_{k,3})\end{aligned} \tag{24}$$

In a matrix form:

$$\begin{pmatrix} a^+_{k,1} & a^+_{k,2} & a^+_{k,3} \end{pmatrix} \begin{pmatrix} \epsilon_k & -t_\perp & -t_\perp \\ -t_\perp & \epsilon_k & -t_\perp \\ -t_\perp & -t_\perp & \epsilon_k \end{pmatrix} \begin{pmatrix} a_{k,1} \\ a_{k,2} \\ a_{k,3} \end{pmatrix} = \begin{pmatrix} c^\dagger_{k,1} & c^+_{k,2} & c^+_{k,3} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \begin{pmatrix} c_{k,1} \\ c_{k,2} \\ c_{k,3} \end{pmatrix}$$

$$\begin{vmatrix} \epsilon_k - \lambda & -t_\perp & -t_\perp \\ -t_\perp & \epsilon_k - \lambda & -t_\perp \\ -t_\perp & -t_\perp & \epsilon_k - \lambda \end{vmatrix} = 0 \tag{25}$$

Expanding along the first row one obtains:

$$(\epsilon_k - \lambda)((\epsilon_k - \lambda)^2 - t_\perp{}^2) + t_\perp(-t_\perp(\epsilon_k - \lambda) - t_\perp{}^2) - t_\perp(t_\perp{}^2 + t_\perp(\epsilon_k - \lambda) = 0 \tag{26}$$

The common factor is $\epsilon_k - \lambda + t_\perp$, so we have a quadratic equation:

$$(\epsilon_k - \lambda + t_\perp)((\epsilon_k - \lambda)(\epsilon_k - \lambda - t_\perp) - 2{t_\perp}^2) = 0 \tag{27}$$

Let's rewrite the second part of the equation with a new variable $\phi = \epsilon_k - \lambda$:

$$\phi^2 - t_\perp \phi - 2{t_\perp}^2 = 0$$

$$D = {t_\perp}^2 + 8{t_\perp}^2 = 9{t_\perp}^2$$

$$\phi_{1,2} = \frac{t_\perp \pm 3t_\perp}{2}$$

Then our final answer for λ is:

$$\lambda_1 = \epsilon_k + t_\perp$$

$$\lambda_2 = \epsilon_k + t_\perp$$

$$\lambda_3 = \epsilon_k - 2t_\perp$$