Density-Functional Formulation for Quantum Chains

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Overview

1. Derivation of DFT-LDA equations
2. Application to the XXZ
3. Conclusions

Derivation of DFT + LDA equations

Operators attached on sites $i = 1, \ldots, L$

$H = T + V^{\text{int}} + V^{\text{ext}} = H_0 + V^{\text{ext}}, \quad V^{\text{ext}} = \sum_{i=1}^{L} v_i^{\text{ext}} \hat{n}_i$

$$\hat{N} = \sum_i^L \hat{n}_i, \quad [H, \hat{N}] = 0, \quad N = 0, 1, 2, \ldots$$

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Example: the XXZ quantum chain

$$H^{\text{XXZ}}(\Delta) = H^{\text{XXZ}}(\Delta) + V^{\text{ext}}$$

$$H^{\text{XXZ}} = -\frac{1}{2} \sum_{j=1}^{L} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) \quad V^{\text{ext}} = \frac{1}{2} \sum_{j=1}^{L} h_j^{\text{ext}} (\sigma_j^z + 1)$$

$$S^z = \sum_{j=1}^{L} \sigma_j^z, \quad [S^z, H^{\text{XXZ}}] = 0$$

How to calculate the ground-state energy E_0 ?

Exact calculation :quite difficult!

$$H|\Psi_0^{(N)}>= E_0|\Psi_0^{(N)}>$$

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$$N = \sum_{i=1}^{N} n_i \quad \text{fixed}$$

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Two steps (Levi, Lieb):

- Minimize over $\{|\Psi>\}$ that produces a fixed density $n(\vec{r}) = (n_1, n_2, \ldots, n_l)$
- Minimize over all possible $\{n(\vec{r})\}$ with fixed $N = \sum_i n_i$

First step:

Ensemble of states $\{|\Psi>\}_{n_1,\dots,n_L}$ such that $<\Psi|\hat{n}_i|\Psi>= n_i$ $(i = 1,\dots,L)$.
Minimize $<\Psi|H_0 + V^{ext}|\Psi>$,

$$\text{Since} \qquad V^{ext} = \sum_{i=1}^{L} v_i^{ext}\hat{n}_i$$

$$\min_{|\Psi>_{n_1,\dots,n_L}} <\Psi|H|\Psi>= F_l[n] + \sum_{i=1}^{L} v_i^{\text{ext}} n_i,$$

with

$$\text{Functional} \rightarrow F_l[n] = \min_{|\Psi>_{n_1,\dots,n_L}} <\Psi|H_0|\Psi>$$

First step:

$$\min_{|\Psi>_{n_1,\ldots,n_L}} < \Psi|H|\Psi >= F_I[n] + \sum_{i=1}^{L} v_i^{\text{ext}} n_i,$$

Functional $\rightarrow F_I[n] = \min_{|\Psi>_{n_1,\ldots,n_L}} < \Psi|H_0|\Psi >$

Second step:

Minimize over all densities (μ is a Lagrange multiplier)

$$\delta \left[F_I[n] + \sum_{i=1}^{L} v_i^{\text{ext}} n_i - \mu \sum_{i=1}^{L} n_i \right] = 0 \rightarrow [n_0]$$

$$E_0 = F_I[n_0]$$

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- How to obtain $F_l[n]$?

Introduce a solvable Hamiltonian (Kohn-Sham)

$$H_s = H_0^s + \sum_{i=1}^{L} v_i^s \hat{n}_i,$$

solvable for arbitrary v_i^s

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$$E_0 = \min_{|\Phi>} < \Phi^{(N)}|H_s|\Phi^{(N)} >=< \Phi_0^{(N)}|H_s|\Phi_0^{(N)} >$$

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Functional $\rightarrow F_s[n] = \min_{|\Phi>_{n_1,\ldots,n_L}} < \Phi|H_0^s|\Phi >$

Second step:

Minimize over all densities (μ_s is a Lagrange multiplier)

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Comparing the Euler-type equations

$$\delta\left[F_l[n]+\sum_{i=1}^{L}v_i^{\text{ext}}n_i-\mu\sum_{i=1}^{L}n_i\right]=0\rightarrow[n_0]$$

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Impose the same density distribution:

$$\rightarrow \sum_{i=1}^{L} v_i^{s} n_i=\sum_{i=1}^{L} v_i^{\text{ext}} n_i+W[n]+(\mu-\mu^s)N$$

where

$$W[n]=F_l[n]-F_s[n]$$

This implies

$$v_i^s=v_i^{\text{ext}}+\frac{\partial W[n]}{\partial n_i}+\mu-\mu^s$$

For a given site $\rightarrow$ v_i^s depends $n_1, \ldots, n_L$

Solve consistently for $n_1, \ldots, n_L$

$$H_s = H_0^s + \sum_{i=1}^{L} v_i^s \hat{n}_i$$

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Success depends on good $F_I[n]$, $F_s[n]$, $W[n]$

In *ab initio* Density-Function Formulation (DFT)

$$F_I[n] = T_s[n] + E_H[n] + E_{xc}[n]$$

In our case

$$F_I[n] = F_s[n] + W[n]$$

$$W(n_1, \ldots, n_L) = \sum_{i=1}^{L} w_i$$

Expanding around the homogeneous distribution

$$w_i = \frac{W(n_i, \ldots, n_i)}{L} + \sum_{j=1}^{L} \alpha_j[n_i](n_j - n_i) + \sum_{j=1}^{L} \sum_{l=1}^{L} \beta_{j,l}[n_i](n_j - n_i)(n_l - n_i) + \cdots$$

$$\alpha_j[n_i] = \frac{1}{L} \frac{\partial W(n_1, \ldots, n_L)}{\partial n_j} \Bigg|_{n_1 = \cdots = n_L = n_i}$$

$$\beta_{j,l}[n_i] = \frac{1}{2L} \frac{\partial^2 W}{\partial n_j \partial n_l} \Bigg|_{n_1 = \cdots = n_L = n_i}$$

Local-Density Approximation (LDA)

$$W^{\mathrm{LDA}}(n_1,\ldots,n_L) = F_I^{\mathrm{LDA}}(n_1,\ldots,n_L) - F_s^{\mathrm{LDA}}(n_1,\ldots,n_L) = \sum_{i=1}^{L} \frac{W(n_i,n_i,\ldots,n_i)}{L}$$

$$F_I^{\mathrm{LDA}}(n_1,\ldots,n_L) = \sum_{i=1}^{L} \frac{F_I^{\mathrm{LDA}}(n_i,n_i,\ldots,n_i)}{L}$$

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$$F_s^{\mathrm{LDA}}(n_1,\ldots,n_L) = \sum_{i=1}^{L} \frac{F_s^{\mathrm{LDA}}(n_i,n_i\ldots,n_i)}{L}$$

$$F_I^{\mathrm{LDA}}(n_i,n_i\ldots,n_i) = \min_{|\Psi>_{n_i,\ldots,n_i}} \frac{<\Psi|H_0|\Psi>}{L} \approx \frac{E_0^{(L)}(n_i)}{L} = e_0^{(L)}(n_i)$$

$$F_s^{\mathrm{LDA}}(n_i,n_i\ldots,n_i) = \min_{|\Phi>_{n_i,\ldots,n_i}} \frac{<\Psi|H_0^s|\Phi>}{L} \approx \frac{E_s^{(L)}(n_i)}{L} = e_s^{(L)}(n_i)$$

General LDAs

$$F_X^{\mathrm{LDA},\infty}(n_1,\ldots,n_L) = \sum_{i=1}^{L} e_X^{(\infty)}(n)|_{n=n_i}, \quad X = \mathrm{l}, s \qquad \infty \quad LDA$$

$$F_X^{\mathrm{LDA,L}}(n_1,\ldots,n_L) = \sum_{i=1}^{L} e_X^{(L)}(n)|_{n=n_i}, \quad X = \mathrm{l}, s \qquad L - finite \quad \mathrm{LDA}$$

$$W^{\mathrm{LDA},\infty}(n_1,\ldots,n_L) = \sum_{i=1}^{L} w^{\infty}(n)|_{n=n_i} \qquad \infty \quad LDA$$

$$W^{\mathrm{LDA,L}}(n_1,\ldots,n_L) = \sum_{i=1}^{L} w^{(L)}(n)|_{n=n_i} \qquad L - finite \quad \mathrm{LDA}$$

Application to the XXZ chain

$$H^{\text{XXZ}}(\Delta) = H_0^{\text{XXZ}}(\Delta) + V^{\text{ext}},$$

$$H^{\text{XXZ}} = -\frac{1}{2}\sum_{j=1}^{L}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z)$$

$$V^{\text{ext}} = \frac{1}{2}\sum_{j=1}^{L} h_j^{\text{ext}}(\sigma_j^z + 1)$$

$$S^z = \sum_{j=1}^{L}\sigma_j^z, \quad [S^z, H^{\text{XXZ}}] = 0$$

Critical for $-1 \leq \Delta = -\cos\gamma \leq 1$

$$x_{n,m} = n^2 x_\Delta + \frac{m^2}{4x_\Delta}, \quad n, m = 0, \pm 1, \pm 2, \ldots$$

$$x_\Delta = \frac{\pi - \gamma}{2\pi}, \quad \Delta = -\cos\gamma, \quad 0 \leq \gamma \leq \pi$$

Kohn-Sham Hamiltonian (XY model)

$$H_s(\{h_i^s\}) = -\frac{1}{2}\sum_{j=1}^{L}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y) - \sum_{j=1}^{L} h_j^s \hat{n}_j, \qquad \hat{n}_j = (\sigma_j^z + 1)/2$$

Same distribution provide

$$h_i^s = h_i^{\text{ext}} - \frac{\partial W[n]}{\partial n}, \quad i = 1, \ldots, L; \qquad W[n] = F_\Delta[n] - F_0[n]$$

$$F_\Delta[n] = \min_{|\Psi>_{n_1,\ldots,n_l}} < \Psi|H_0^{\text{xxz}}(\Delta)|\Psi >$$

Local approximations - Periodic boundaries Homogeneous LDA

$$F_\Delta[n] = \min_{|\Psi>_{n_1,\dots,n_L}} < \Psi | H_0^{\mathrm{XXZ}}(\Delta) | \Psi >$$

$$W_\Delta(n_1,\dots,n_L) = F_\Delta(n_1,\dots,n_L) - F_0(n_1,\dots,n_L)$$

$$n_i = \frac{N}{L} \quad (i = 1,\dots,L), \qquad F_\Delta[n] = F_\Delta(n) \quad \text{simple function}$$

Translation invariance: momentum p is a good quantum number

$$p = \frac{2\pi}{j}, j = 0,\dots,L-1$$

$$W_\Delta^{\mathrm{LDA},L}(n,p) = \sum_{i=1}^{L} w_\Delta^{L,\mathrm{per}}(n,p) = L w_\Delta^{L,\mathrm{per}}(n,p) \quad \rightarrow \text{exact result}$$

$$W_\Delta^{\mathrm{LDA},\infty}(n,p) = \sum_{i=1}^{L} w_\Delta^{\infty}(n,p) = L w_\Delta^{\infty}(n,p). \quad \rightarrow \text{non exact}$$

$W_\Delta^\infty(n,p)$ is correct $o(1/L)$? (conformal anomaly, critical exponents?)

Exact conformal invariance prediction: $E_\Delta^{\text{per}}(L,n,p)$ (g. state $\rightarrow n=\frac{1}{2}, p=0$)

$$E_\Delta^{\text{per}}(L;\frac{1}{2},0) = Le_\Delta^\infty(\frac{1}{2},0) - \frac{\pi v_\Delta c_\Delta}{6L} + o(\frac{1}{L}),$$

$$c_\Delta = 1, \quad v_\Delta = \frac{\pi \sin\gamma}{\gamma}, \quad \Delta = -\cos\gamma$$

LDA - ∞ prediction

$$E_\Delta^{\text{LDA},\infty}(L;\frac{1}{2},0) = Le_\Delta^\infty(\frac{1}{2},0) - \pi c_\Delta v_0/6L + o(\frac{1}{L})$$

wrong results for $o(1/L)$ ($v_0 = 2 \neq v_\Delta$)

Gaps predictions - sectors $n = \frac{n}{L} = \frac{1}{2} + \frac{\nu}{L}$ $(\nu = \pm 1, \pm 2)$

Exact conformal invariance prediction:

$$G_L^{\nu} = E_{\Delta}(L; \frac{1}{2} + \frac{\nu}{L}, 0) - E_{\Delta}(L; \frac{1}{2}, 0) = \frac{2\pi}{L} v_{\Delta} x_{\Delta} \nu^2 + o(\frac{1}{L})$$

Exact conformal invariance prediction:

$$G_L^{p} = E_{\Delta}(L; \frac{1}{2}, p) - E_{\Delta}(L; \frac{1}{2}, 0) = v_{\Delta} p + o(\frac{1}{L})$$

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LDA -∞ results

$$G_L^{\text{LDA},\nu} = \frac{2\pi}{L} v_{\Delta} x_{\Delta} \nu^2 + o(\frac{1}{L}), \quad \nu = \pm 1, \pm 2, \dots$$

correct critical exponents

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LDA -∞ results

$$G_L^{\text{LDA,p}} = v_0 p, \qquad v_0 = 2 \tag{1}$$

wrong sound velocity v_{Δ}

Instead of $H^{\mathrm{XXZ}}(\Delta)$ consider

$$H = H^{\mathrm{XXZ}}(\Delta)/v_{\Delta}$$

WE OBTAIN CORRECT PREDICTIONS FOR c_{Δ} AND v_{Δ} !

XXZ - Open boundary conditions

In general $n_1, n_2, \ldots, n_l$ inhomogenous

Exception: sector $\sum_{i=1}^{L} \sigma_i^z = 0$

$$n_i = < \Psi|(\sigma_i^z + 1)/2|\Psi > / < \Psi|\Psi > = \frac{1}{2}, \quad i = 1, \ldots, L$$

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$$n_i =< \Psi|(\sigma_i^z + 1)/2|\Psi > / < \Psi|\Psi >= \frac{1}{2}, \quad i = 1, \ldots, L$$

Exact conformal invariance predictions

$$E_\Delta^{\text{open}}(L, \frac{1}{2}) = Le_\Delta^\infty(\frac{1}{2}) + f_\Delta^s - \frac{\pi c_\Delta v_\Delta}{24L} + o(\frac{1}{L})$$

$$G_L^{\nu,\text{open}} = E_\Delta^{\text{open}}(L, \frac{1}{2} + \frac{\nu}{L}) - E_\Delta^{\text{open}}(L, \frac{1}{2}) = \frac{\pi}{L} v_\Delta x_\Delta^{s,\nu} + o(\frac{1}{L})$$

$x_\Delta^{s,\nu} = 2x_\Delta \nu^2 \leftarrow$ surface critical exponents

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LDA for the ground state (homogeneous distribution)

$$E^{\text{LDA},\infty}(L, \frac{1}{2}) = Le_\Delta^\infty(\frac{1}{2}) + [f_0^s - e_\Delta^\infty(\frac{1}{2}) + e_0^\infty(\frac{1}{2})] - \frac{\pi c_0 v_0}{24L} + o(\frac{1}{L})$$

Wrong results for f_s and v_Δ

How to fix this?

$f^s_\Delta, v_\Delta, e^\infty_\Delta$ are non universal

CFT $\longrightarrow$ fixed vacuum energy, sound velocity, conformal anomaly

$$\tilde{H}^{xxz}(\Delta) = (H^{xxz}(\Delta) - Le^\infty_\Delta - f^s_\Delta)/v_\Delta$$

Open boundary conditions (other sectors)

Non local functionals

$$W_{\Delta}^{\mathrm{LDA},\infty}(n_1,\ldots,n_L) =$$
$$\frac{L-1}{L}\left[\sum_{i=1}^{L} w_{\Delta}^{\infty}(n_i) + \frac{1}{4}\sum_{i=1}^{L}(2-\delta_{i,1}-\delta_{i,L})(\frac{N}{L}-n_i)\frac{\partial w_{\Delta}^{\infty}}{\partial n}(n)\bigg|_{n=n_i}\right]$$

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How to obtain $w_{\Delta}^{\infty} = Le_{\Delta}^{\infty}(n) - Le_{0}^{\infty}(n)$?

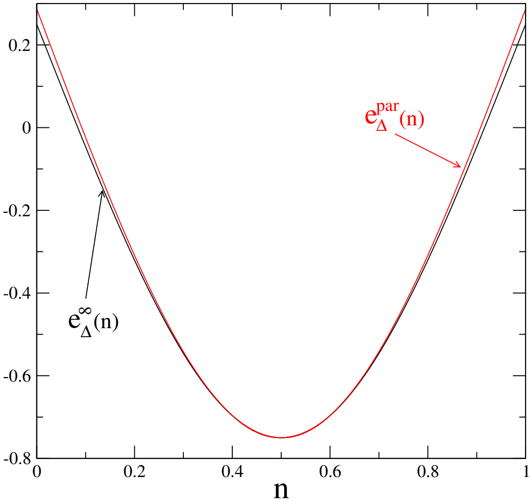
- Solve the Bethe ansatz equations (integral equations for each n)

OR

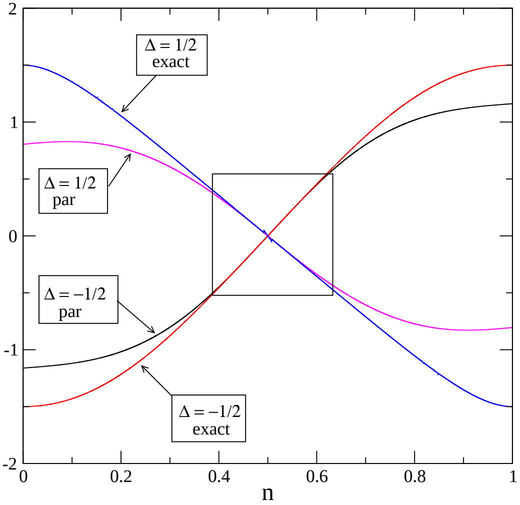
- Produce an analitical approximation: $e_{\Delta}^{\mathrm{par}}$

Using the exact solution and conformal invariance predictions for finite-size corrections

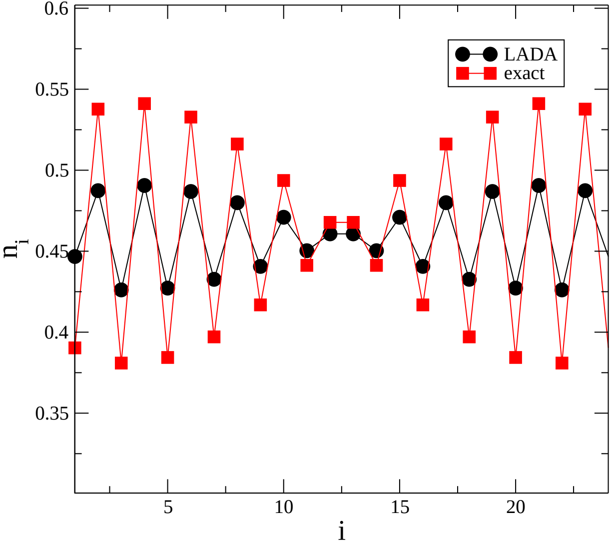
Comparison of $e_\Delta^{par}(n)$ with the exact $e_\Delta^{\infty}(n)$, at $\Delta = -1/2$



Comparison of effective field $h^s = h^s_1 = \cdots = h^s_L$



Exact and LDA predictions of n_i at $\Delta = -\frac{1}{2}$ of lowest eigenstate in sector $N = 11$ for $L = 24$



Exact and LDA results of eigenenergies for $L = 1, \ldots, 24$ at $\Delta = -\frac{1}{2}$

L	$E_{\Delta}^{\text{open}}(L, \frac{1}{2})$	$E^{\text{LDA}}(L, \frac{1}{2})$	$E_{\Delta}^{\text{open}}(L, \frac{1}{2} + \frac{1}{L})$	$E^{\text{LDA}}(L, \frac{1}{2} + \frac{1}{L})$
4	-0.678043	-0.644052	-0.437500	-0.387850
6	-0.699296	-0.676810	-0.581496	-0.549768
8	-0.710812	-0.694054	-0.640983	-0.618987
10	-0.718050	-0.704710	-0.671853	-0.655200
12	-0.723025	-0.711951	-0.690197	-0.676901
14	-0.726656	-0.717194	-0.702125	-0.691102
16	-0.729424	-0.721166	-0.710396	-0.700999
18	-0.731604	-0.724279	-0.713276	-0.708232
20	-0.733365	-0.726786	-0.720956	-0.713716
22	-0.734819	-0.728847	-0.724490	-0.717998
24	-0.736039	-0.730572	-0.727307	-0.721423

LDA results of eigenenergies for $L = 16, \ldots, 1424$ at $\Delta = -\frac{1}{2}$

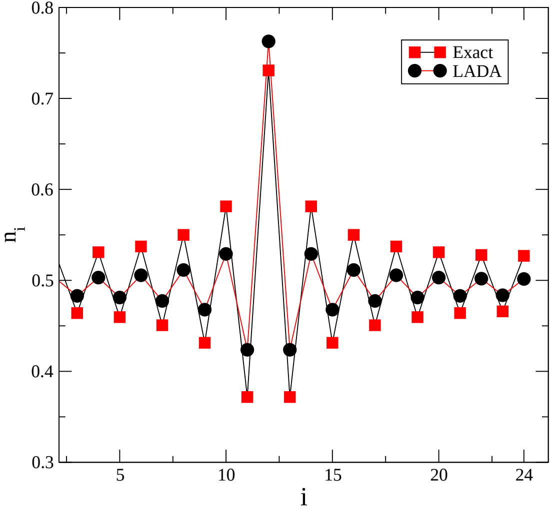
L	$E_\Delta^{\mathrm{LDA}}(L, \frac{1}{2})/L$	$E_\Delta^{\mathrm{LDA}}(L, \frac{1}{2} + \frac{1}{L})/L$	$E_\Delta^{\mathrm{LDA}}(L, \frac{1}{2} + \frac{2}{L})/L$
16	-0.721166	-0.700999	-0.641516
32	-0.735349	-0.730155	-0.714603
64	-0.742614	-0.741299	-0.737349
128	-0.746291	-0.745961	-0.744968
256	-0.748142	-0.748059	-0.747810
512	-0.749070	-0.749049	-0.748987
1024	-0.749535	-0.749529	-0.749513
1224	-0.749611	-0.749607	-0.749596
1424	-0.749665	-0.749663	-0.749655
∞ (exact)	-0.75	-0.75	-0.75

LDA results of gaps at $\Delta = -\frac{1}{2}$

L	$G^{\text{LDA}}_{L,\nu=1} L^2/\pi$	$G^{\text{LDA}}_{L,\nu=2} L^2/\pi$	ratio
16	1.643310	6.490450	3.949620
32	1.693019	6.762162	3.994144
64	1.714280	6.863298	4.003604
128	1.723679	6.901329	4.003837
256	1.728007	6.916386	4.002522
512	1.730070	6.922749	4.001427
1024	1.731081	6.925648	4.000765
1224	1.731302	6.926084	4.000506
1424	1.731408	6.928203	4.000439
∞ (exact)	1.732051	6.928203	4

$G^{\text{LDA}}_{L,\nu=1} L^2/\pi \rightarrow x_\Delta = 1.732051 \quad G^{\text{LDA}}_{L,\nu=2} L^2/\pi \rightarrow 4x_\Delta = 6.928203$

Periodic chain with an impurity $h_i^{ext} = \delta_{i,11}$ for $L = 24, N = 12$ and $\Delta = -\frac{1}{2}$



From conformal invariance: the average gap

$$\bar{G}_L^{\nu,\text{per}} = \frac{1}{2}[E_\Delta^{\text{per}}(L, \frac{1}{2} + \frac{\nu}{L}) + E_\Delta^{\text{per}}(L, \frac{1}{2} - \frac{\nu}{L}) - 2E_\Delta^{\text{per}}(L, \frac{1}{2})] = \frac{\pi}{L} v_\Delta x_\Delta^{s,\nu} + o(\frac{1}{L}),$$

$$x_\Delta^{s,\nu} = 2x_\Delta \nu^2 \quad \text{surface exponents} \tag{2}$$

Values at $\Delta = -1/2$

L	$E_\Delta^{\text{per}}(L, \frac{1}{2})$	$L\bar{G}_L^{1,\text{per}}\pi$	$L\bar{G}_L^{2,\text{per}}\pi$	$\bar{G}_L^{2,\text{per}}/\bar{G}_L^{1,\text{per}}$
8	-0.736502	1.646049	6.211188	3.773392
16	-0.738800	1.685301	6.657321	3.950226
32	-0.743287	1.707394	6.816070	3.992090
64	-0.746363	1.719601	6.879476	4.000623
128	-0.748111	1.725632	6.905708	4.001843
256	-0.749038	1.728826	6.917514	4.001278
512	-0.749515	1.730444	6.923041	4.000730
1024	-0.749756	1.731253	6.925686	4.000389
∞ (exact)	-0.75	1.732051	6.928204	4

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- Application to other non-integrable models in $d = 1$.
- Quantum Hamiltonians in $d = 2$ and $d = 3$?