Exact surface energy of the Hubbard model with unparallel boundary magnetic fields

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Outline

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1. Bethe ansatz solutions
2. Patterns of Bethe Roots
3. Contribution of inhomogenous terms
4. Surface energy

(1)Bethe ansatz solutions

Bethe ansatz solutions

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We investigate the Hubbard chain with **general boundary fields**

$$H = -t \sum_{\alpha=\uparrow,\uparrow} \sum_{j=1}^{N-1} [c_{j,\alpha}^{\dagger} c_{j+1,\alpha} + c_{j+1,\alpha}^{\dagger} c_{j,\alpha}] + U \sum_{j=1}^{N} n_{j\uparrow} n_{j\downarrow} + h_1^z (n_{1,\uparrow} - n_{1,\downarrow}) + h_N^z (n_{N,\uparrow} - n_{N,\downarrow})$$

$$+h_1^- c_{1,\uparrow}^+ c_{1,\downarrow} + h_1^+ c_{1,\downarrow}^+ c_{1,\uparrow} + h_N^- c_{N,\uparrow}^+ c_{N,\downarrow} + h_1^+ c_{N,\downarrow}^+ c_{N,\uparrow} +$$

- $c_{j,\alpha}^+$ and $c_{j,\alpha}$ are the creation and annihilation operators
- t, $n_{j,\alpha}$ and U are hopping constant, the number of electrons and on-site repulsive interaction
- the unparallel boundary fields **break the U (1) symmetry** and the z-component of the total spin is no longer a good quantum number

general boundary magnetic fields

Bethe ansatz solutions

Combining the **coordinate and off-diagonal Bethe ansatz methods**, the eigen-energy E of the Hamiltonian can be expressed by

Y.-Y Li et al, Nucl. Phys. B 879 (2014) 98.

$$E = -2t\sum_{j=1}^{\bar{M}} \cos k_j,$$

where the quasi-momenta k_j satisfy the inhomogeneous BAEs

inhomogenous term

$$\frac{4(p-\sin k_j\varepsilon|\mathbf{h}_N|)}{1-\mathbf{h}_1^2 e^{2ik_j}}\frac{(q+\sin k_j|\mathbf{h}_1|)}{e^{-2ik_j}-\mathbf{h}_N^2} = e^{-2ik_jN}\prod_{l=1}^{M}\frac{(\sin k_j+\lambda_l-\frac{\eta}{2})}{(\sin k_j+\lambda_l+\frac{\eta}{2})}\frac{(\sin k_j-\lambda_l-\frac{\eta}{2})}{(\sin k_j-\lambda_l+\frac{\eta}{2})},$$

$$j = 1,\cdots,\bar{M},$$

$$\frac{\lambda_j+\frac{\eta}{2}}{\lambda_j-\frac{\eta}{2}}\frac{p+(\lambda_j-\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}{p-(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}\frac{q-(\lambda_j-\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}{q+(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}\prod_{l=1}^{\bar{M}}\frac{\lambda_j+\sin k_l+\frac{\eta}{2}}{\lambda_j+\sin k_l-\frac{\eta}{2}}\frac{\lambda_j-\sin k_l+\frac{\eta}{2}}{\lambda_j-\sin k_l-\frac{\eta}{2}} =$$

$$\prod_{l=1}^{M}\frac{\lambda_j-\lambda_l+\eta}{\lambda_j-\lambda_l-\eta}\frac{\lambda_j+\lambda_l+\eta}{\lambda_j+\lambda_l-\eta} - c\frac{\lambda_j+\frac{\eta}{2}}{p-(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}\frac{2\lambda_j}{q+(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}$$

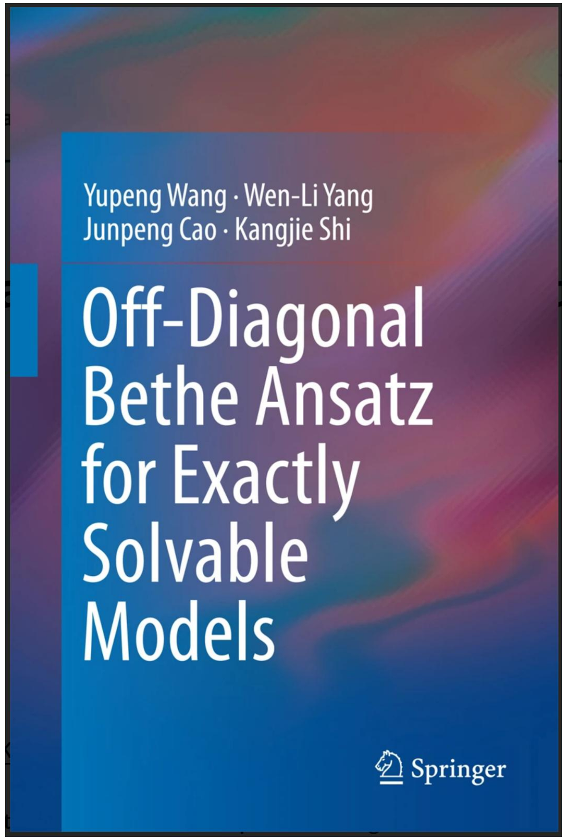
$$\times\prod_{l=1}^{\bar{M}}\frac{(\lambda_j+\sin k_l+\frac{\eta}{2})}{(\lambda_j-\lambda_l+\eta)}\frac{(\lambda_j-\sin k_l+\frac{\eta}{2})}{(\lambda_j+\lambda_l-\eta)}, \qquad j = 1,\cdots,M,$$

$$\varepsilon = \frac{\mathbf{h}_1.\mathbf{h}_N}{|\mathbf{h}_1.\mathbf{h}_N|}$$

$$c = 2(\varepsilon|\mathbf{h}_1||\mathbf{h}_N| - \mathbf{h}_1.\mathbf{h}_N).$$

Bethe ansatz solutions

About the off-diagonal Bethe ansatz methods



where

$$\bar{\tau}(k_j) = S_{j-1,j}(k_{j-1},k_j)\cdots S_{1,j}(k_1,k_j)\bar{K}_j^{+}(k_j)S_{j,1}(-k_j,k_1)\cdots \\ \times S_{j,j-1}(-k_j,k_{j-1})S_{j,j+1}(-k_j,k_{j+1})\cdots S_{j,M}(-k_j,k_M)\bar{K}_j^{-}(k_j) \\ \times S_{M,j}(k_M,k_j)\cdots S_{j+1,j}(k_{j+1},k_j). \quad (6.2.16)$$

6.2.2 *Off-Diagonal Bethe Ansatz*

Let us introduce the K-matrices

$$K^{-}(u) = \bar{p} + u\,\mathbf{h}_N\cdot\boldsymbol{\sigma}, \quad (6.2.17)$$

$$K^{+}(u) = \bar{q} - (u+\eta)\mathbf{h}_1\cdot\boldsymbol{\sigma}, \quad (6.2.18)$$

with

$$\bar{p} = i\frac{\mathbf{h}_N^2 - t^2}{2t}, \quad \bar{q} = i\frac{t^2 - \mathbf{h}_1^2}{2t}.$$

The following RE and its dual equation hold:

$$R_{0,\bar{0}}(u-v)K_0^{-}(u)R_{\bar{0},0}(u+v)K_{\bar{0}}^{-}(v) \\ = K_{\bar{0}}^{-}(v)R_{0,\bar{0}}(u+v)K_0^{-}(u)R_{\bar{0},0}(u-v), \quad (6.2.19)$$

$$R_{0,\bar{0}}(v-u)K_0^{+}(u)R_{\bar{0},0}(-u-v-2\eta)K_{\bar{0}}^{+}(v) \\ = K_{\bar{0}}^{+}(v)R_{\bar{0},0}(-u-v-2\eta)K_0^{+}(u)R_{\bar{0},0}(v-u), \quad (6.2.20)$$

where the R-matrix is given by (6.1.20). To solve the eigenvalue problem (6.2.16), let us introduce the inhomogeneous double-row monodromy matrix

$$\mathscr{U}_0(u) = R_{0,1}(u-\sin k_1)\cdots R_{0,M}(u-\sin k_M)K_0^{-}(u) \\ \times R_{M,0}(u+\sin k_M)\cdots R_{1,0}(u+\sin k_1), \quad (6.2.21)$$

and the transfer matrix $\tau(u)$,

$$\tau(u) = tr_0\{K_0^{+}(u)\mathscr{U}_0(u)\}. \quad (6.2.22)$$

Noting that

$$\bar{K}_j^{-}(k_j) = it\frac{2K_j^{-}(-\sin k_j)}{\mathbf{h}_N^2 - t^2e^{-2ik_j}}, \quad (6.2.23)$$

(2)Patterns of Bethe Roots

Patterns of Bethe roots

Here we consider the singularity of BAEs, the singular points of BAEs are

$$\frac{1-|\mathbf{h}|^2}{2|\mathbf{h}|}-\frac{U}{4}, \quad \mathbf{h}=\mathbf{h}_1,\mathbf{h}_N.$$

- Critical point $|\mathbf{h}| = 1$ characterizes the **periodic structure** of the scattering process of the quasi-particles

- If $\frac{1-h_0^2}{2h_0}-\frac{U}{4}=0.$ The resulted energy is the surface energy induced by the **free open boundary** (open, but without boundary fields).

$$\frac{\lambda_j - i(\frac{1-\beta^2}{2\beta}-\frac{U}{4})}{\lambda_j + i(\frac{1-\beta^2}{2\beta}-\frac{U}{4})}\frac{\lambda_j - i(\frac{1-\alpha^2}{2\alpha}-\frac{U}{4})}{\lambda_j + i(\frac{1-\alpha^2}{2\alpha}-\frac{U}{4})}$$

Patterns of Bethe roots

According to the singular points, we conclude that the boundary parameters can be divided into **five regions**:

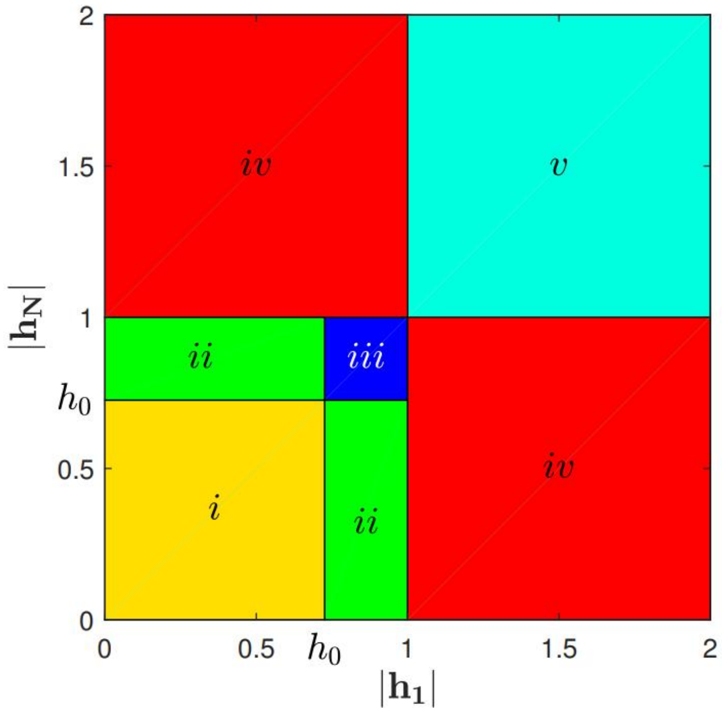


FIG. 2. The different regions of the boundary parameters in the $\mathbf{h}_1$-$\mathbf{h}_N$ plane at the ground state. The configuration of Bethe roots in different regions are different. Here $U = 1.3$.

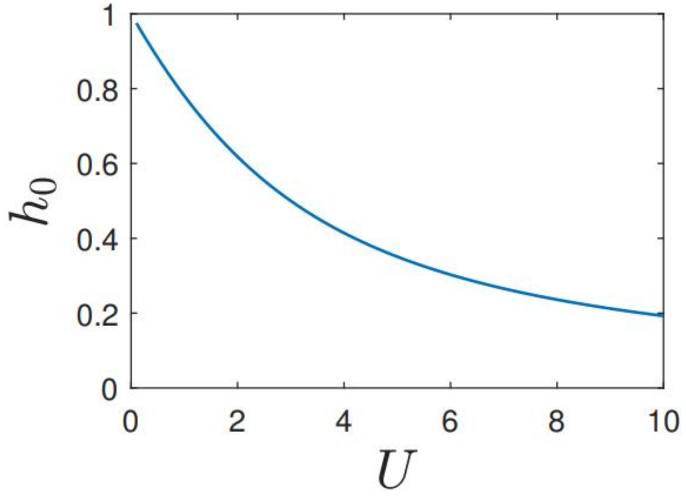


FIG. 1. The value of critical field h_0 versus the on-site coupling U. h_0 satisfies $(h_0^2 - 1)/2h_0 + U/4 = 0$ and $h_0 > 0$.

Patterns of Bethe roots

In the different regions of boundary parameters, the **patterns of Bethe roots** in the reduced BAEs are different, which are summarized

TABLE I. The patterns of Bethe roots at the ground state in different regions, where N is the number of electrons and M is the number of the Bethe roots, $\alpha = |\mathbf{h}_1|$ and $\beta = |\mathbf{h}_N|$.

region	$\{k_j \mid j = 1, \cdots, N\}$	$\{\lambda_j \mid j = 1, \cdots, M = \frac{N}{2}\}$	α, β
i	$k_j \in \mathbf{R}$	$\lambda_j \in \mathbf{R}$	$0 < \alpha < h_0 \quad 0 < \beta < h_0$
ii	$k_j \in \mathbf{R}$	$\lambda_j \in \mathbf{R}, j = 1, \cdots, \frac{N}{2} - 1 \quad \lambda_M = i\left(\frac{1-\beta^2}{2\beta} - \frac{U}{4}\right)$	$0 < \alpha < h_0 \quad h_0 < \beta < 1$
iii	$k_j \in \mathbf{R}$	$\lambda_j \in \mathbf{R}, j = 1, \cdots, \frac{N}{2} - 1$ $\lambda_{M-1} = i\left(\frac{1-\alpha^2}{2\alpha} - \frac{U}{4}\right) \quad \lambda_M = i\left(\frac{1-\beta^2}{2\beta} - \frac{U}{4}\right)$	$h_0 < \alpha < 1 \quad h_0 < \beta < 1$
iv	$k_j \in \mathbf{R}, j = 1, \cdots, N-1$ $k_N = \arcsin(i\frac{\beta^2-1}{2\beta})$	$\lambda_j \in \mathbf{R} \quad j = 1, \cdots, \frac{N}{2} - 1$ $\lambda_M = i\left(\frac{\beta^2-1}{2\beta} + \frac{U}{4}\right)$	$0 < \alpha < 1 \quad \beta > 1$
v	$k_j \in \mathbf{R}, j = 1, \cdots, N-2$ $k_{N-1} = \arcsin(i\frac{\alpha^2-1}{2\alpha})$ $k_N = \arcsin(i\frac{\beta^2-1}{2\beta})$	$\lambda_j \in \mathbf{R} \quad j = 1, \cdots, \frac{N}{2} - 2$ $\lambda_{M-1} = i\left(\frac{\alpha^2-1}{2\alpha} + \frac{U}{4}\right) \quad \lambda_M = i\left(\frac{\beta^2-1}{2\beta} + \frac{U}{4}\right)$	$\alpha > \beta > 1$

Patterns of Bethe roots

Why we expect the pattern of Bethe roots would be different in different regions?

Principle: If a Bethe root is the complex number in the upper complex plane, substituting this Bethe root into BAEs, one will find that the left hand side of BAEs tend to infinity (or zero) in the **thermodynamic limit**. Then the right hand side of BAEs must also tend to infinity (or zero) to keep the BAEs hold. For example,

$$\lambda_M = i\left[\frac{1-|\mathbf{h}_N|^2}{2|\mathbf{h}_N|} - \frac{U}{4}\right] + O(N^{-1}).$$

$$\frac{p+(\lambda_j-\frac{\eta}{2})|\mathbf{h}_N|}{p-(\lambda_j+\frac{\eta}{2})|\mathbf{h}_N|}\frac{q-(\lambda_j-\frac{\eta}{2})|\mathbf{h}_1|}{q+(\lambda_j+\frac{\eta}{2})|\mathbf{h}_1|}\frac{\lambda_j+\frac{\eta}{2}}{\lambda_j-\frac{\eta}{2}}\prod_{l=1}^{\bar{M}}\frac{\lambda_j+\sin k_l+\frac{\eta}{2}}{\lambda_j+\sin k_l-\frac{\eta}{2}}\frac{\lambda_j-\sin k_l+\frac{\eta}{2}}{\lambda_j-\sin k_l-\frac{\eta}{2}}$$

$$=\prod_{l=1}^{M}\frac{\lambda_j-\lambda_l+\eta}{\lambda_j-\lambda_l-\eta}\frac{\lambda_j+\lambda_l+\eta}{\lambda_j+\lambda_l-\eta}, \quad j=1,\cdots,M.$$

0

Infinity

(3)Contribution of inhomogenous terms

Contribution of the inhomogenous term

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Why we consider the contribution of the inhomogenous term?

$$\frac{4(p-\sin k_j\varepsilon|\mathbf{h}_N|)}{1-\mathbf{h}_1^2e^{2ik_j}}\frac{(q+\sin k_j|\mathbf{h}_1|)}{e^{-2ik_j}-\mathbf{h}_N^2}=e^{-2ik_jN}\prod_{l=1}^{M}\frac{(\sin k_j+\lambda_l-\frac{\eta}{2})}{(\sin k_j+\lambda_l+\frac{\eta}{2})}\frac{(\sin k_j-\lambda_l-\frac{\eta}{2})}{(\sin k_j-\lambda_l+\frac{\eta}{2})},$$

$$j=1,\cdots,\bar{M},$$

$$\frac{\lambda_j+\frac{\eta}{2}}{\lambda_j-\frac{\eta}{2}}\frac{p+(\lambda_j-\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}{p-(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}\frac{q-(\lambda_j-\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}{q+(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}\prod_{l=1}^{\bar{M}}\frac{\lambda_j+\sin k_l+\frac{\eta}{2}}{\lambda_j+\sin k_l-\frac{\eta}{2}}\frac{\lambda_j-\sin k_l+\frac{\eta}{2}}{\lambda_j-\sin k_l-\frac{\eta}{2}}=$$

$$\prod_{l=1}^{M}\frac{\lambda_j-\lambda_l+\eta}{\lambda_j-\lambda_l-\eta}\frac{\lambda_j+\lambda_l+\eta}{\lambda_j+\lambda_l-\eta}-c\frac{\lambda_j+\frac{\eta}{2}}{p-(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_N|}\frac{2\lambda_j}{q+(\lambda_j+\frac{\eta}{2})\varepsilon|\mathbf{h}_1|}$$

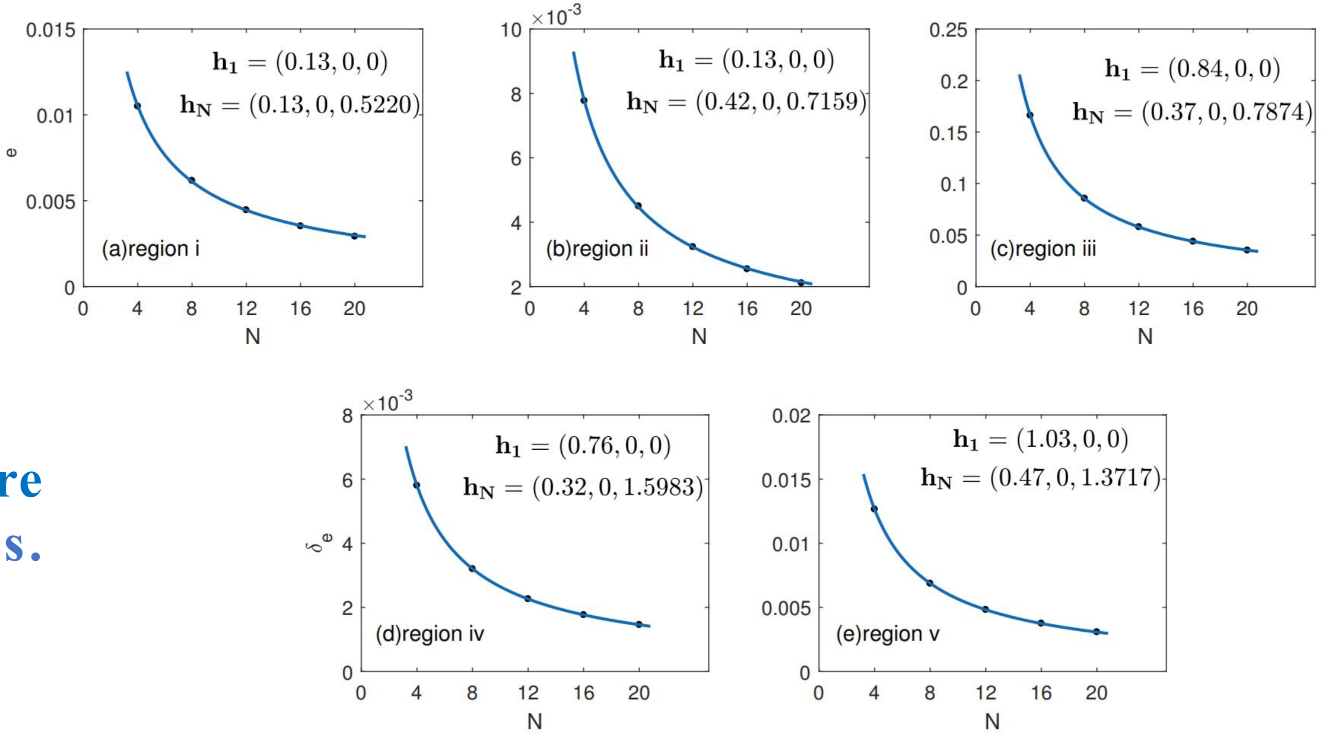
$$\times\prod_{l=1}^{\bar{M}}\frac{(\lambda_j+\sin k_l+\frac{\eta}{2})}{(\lambda_j-\lambda_l+\eta)}\frac{(\lambda_j-\sin k_l+\frac{\eta}{2})}{(\lambda_j+\lambda_l-\eta)},\qquad j=1,\cdots,M,$$

Contribution of the inhomogenous term

$$\delta_e = |E - E_{hom}|.$$

$$E = E_0 + E_b + o(\frac{1}{N}).$$

It is evident that δ_e measures the contribution of the inhomogeneous term. To determine the value of E for given boundary parameters $\mathbf{h}_1 = (h_1^x, h_1^y, h_1^z)$ and $\mathbf{h}_N = (h_N^x, h_N^y, h_N^z)$, we employ the DMRG method. The value of E_{hom} can be obtained using the equivalent parallel boundary fields $|\mathbf{h}_1|\hat{z} = \sqrt{(h_1^x)^2 + (h_1^y)^2 + (h_1^z)^2}\hat{z}$ and $|\mathbf{h}_N|\hat{z} = \sqrt{(h_N^x)^2 + (h_N^y)^2 + (h_N^z)^2}\hat{z}$, where $\hat{z}$ means the unit vector along the z-direction.



Here **ED** and **DMRG** in **Itensor software** are used (**M. Fishman, SciPost Phys. Codebases 004 (2022)**).

By fitting the data, we observe that δe and N exhibit a **power-law relationship**

$$\delta_e = \gamma N^{\tau}.$$

(4)Surface energy

Surface energy

By substituting the distribution of the Bethe roots into the BAEs and using the **Yang-Yang approach**, we obtain the density of the Bethe roots:

$$\rho_s(\mu) = \boxed{\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-i\omega\mu}}{2\cosh\frac{U}{4}|\omega|}J_0(\omega)d\omega +}$$
$$\frac{1}{2N}\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-i\omega\mu}}{2\cosh\frac{U}{4}|\omega|}\int_{-\pi}^{\pi}e^{i\omega\sin k}\left[-b_\alpha(k)-b_\beta(k)-\delta(k)-\frac{1}{2}\delta(k-\pi)-\frac{1}{2}\delta(k+\pi)\right]dkd\omega +$$
$$\frac{1}{2N}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i\omega\mu}\frac{e^{-\frac{U}{4}|\omega|}+e^{\frac{\tilde{U}_\beta}{4}|\omega|}+e^{\tilde{U}_\alpha|\omega|/4}-1-e^{i\omega\infty}-e^{-i\omega\infty}}{1+e^{-U|\omega|/2}}d\omega,$$

$$\rho_c(k) = \boxed{\frac{1}{2\pi}+\frac{\cos k}{2\pi}\int_{-\infty}^{\infty}\frac{e^{i\omega\sin k}e^{-\frac{U}{4}|\omega|}}{2\cosh\frac{U}{4}|\omega|}J_0(\omega)d\omega}$$
$$+\frac{1}{2N}\left[-b_\alpha(k)-b_\beta(k)+d_\alpha(k)+d_\beta(k)-\delta(k)-\frac{\delta(k+\pi)}{2}-\frac{\delta(k-\pi)}{2}\right]$$
$$+\frac{1}{2N}\frac{\cos k}{2\pi}\int_{-\infty}^{\infty}\frac{e^{i\omega\sin k}e^{-\frac{U}{4}|\omega|}}{2\cosh\frac{U}{4}|\omega|}\left(-\tilde{b}_\alpha(\omega)-\tilde{b}_\beta(\omega)+e^{-\frac{U}{4}|\omega|}+e^{\frac{\tilde{U}_\beta}{4}|\omega|}+e^{\frac{\tilde{U}_\alpha}{4}|\omega|}-3-e^{i\omega\infty}-e^{-i\omega\infty}\right)d\omega,$$

Surface energy

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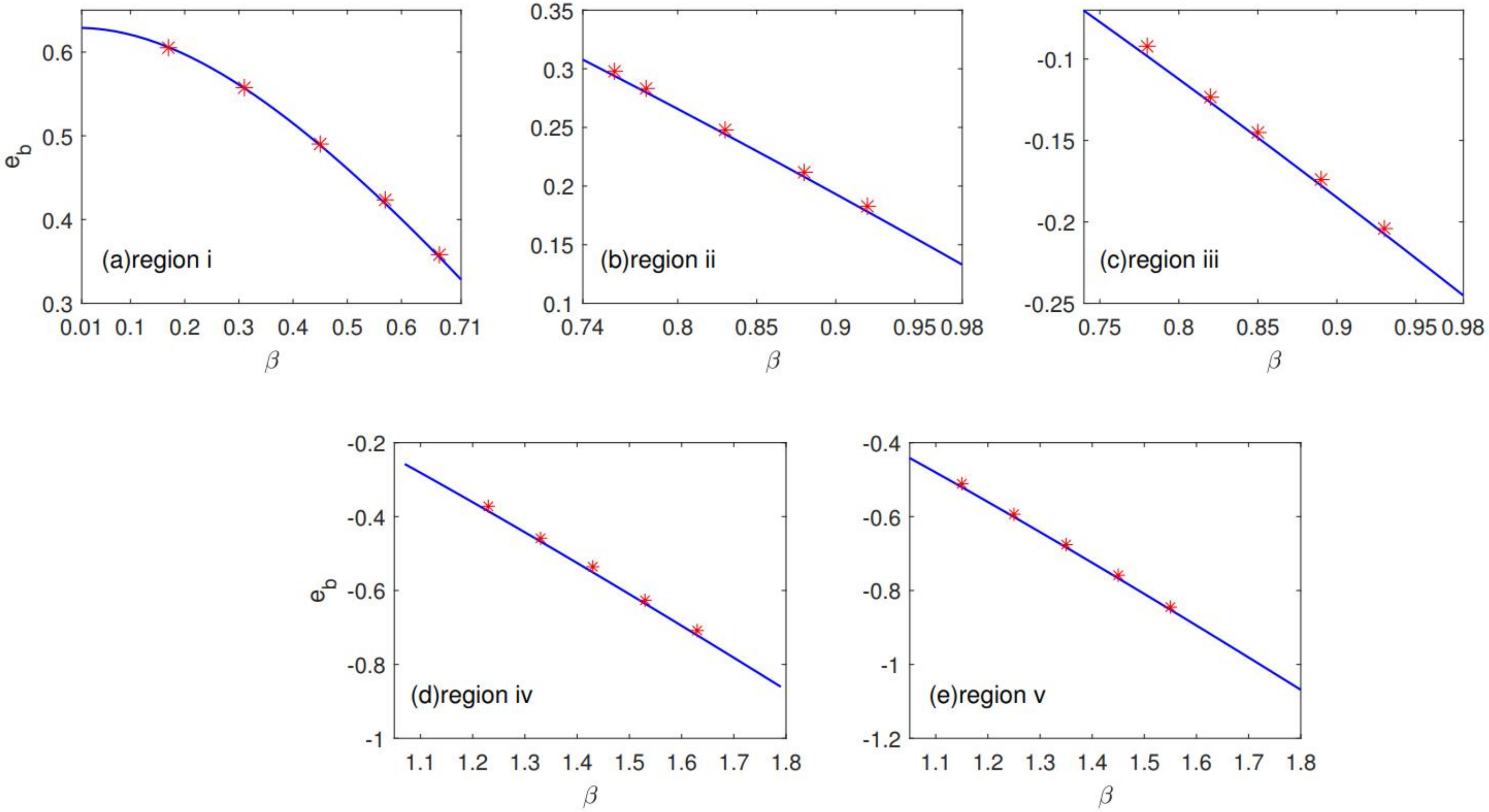
The grund state energy and the surface energy

$$E_g = -2N \int_{-\pi}^{\pi} \cos k \rho_c(k) dk = -4N \int_0^{\infty} \frac{J_0(\omega) J_1(\omega)}{\omega\left(1 + e^{\frac{U\omega}{2}}\right)} d\omega + e_b,$$

$$\begin{aligned} e_b \quad = \quad & -\int_{-\pi}^{\pi} \frac{\cos k^2}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega \sin k}}{1 + e^{\frac{U\omega}{2}}} \left(-\tilde{b}_\alpha(\omega) - \tilde{b}_\beta(\omega)\right) d\omega dk + 2 \int_{-\pi}^{\pi} \frac{\cos k^2}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega \sin k}}{1 + e^{\frac{U\omega}{2}}} d\omega dk \\ & - \int_{-\pi}^{\pi} \frac{\cos k^2}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega \sin k}}{2 \cosh \frac{U}{4}|\omega|} \left[e^{-\frac{U}{4}|\omega|} - 1 - e^{i\omega\infty} - e^{-i\omega\infty} + f_1(\omega, \alpha, \beta)\right] d\omega dk \\ & - \int_{-\pi}^{\pi} \cos k \left[d_\alpha(k) + d_\beta(k) + f_2(k, \alpha, \beta)\right], \end{aligned}$$

Surface energy

We also compute the surface energy using the **DMRG (Itensor software)** approach. The results, depicted **as red stars** , are compared to the surface energies obtained from the **analytical expression** represented by the **blue curves**. **(arXiv:2401.14356)**



Surface energy

Is it reasonable to ignore the inhomogeneous term?

Answer: By analyzing the distribution of **zero roots** of the transfer matrix, they prove exactly that the **inhomogeneous term** contributes nothing to the surface energy to the leading order. (Y. Qiao, et. al, Phys. Rev. B 103 (2021) L220401)

We also note that the **eigenstates** of the system with **non-parallel boundary magnetic** fields are totally different from those with equivalent parallel ones in the thermodynamic limit. The boundary magnetic fields can significantly affect the **spin configurations of electrons** in the bulk. The eigenstates of the system are **helical**, which are quite different from those with parallel boundary fields or periodic boundary conditions.

Thank you for your attention!