DOCTOR THESIS

Non-Hermitian Quantum Mechanics of Strongly Correlated Systems

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Abstract

We conjecture for strongly correlated quantum systems that the imaginary part of a zero of the dispersion relation of the elementary excitation is equal to the inverse correlation length. In order to calculate the dispersion relation and to search zeros in the complex momentum space, we transform the Hermitian Hamiltonian to a non-Hermitian one by replacing the momentum p with $p + \mathrm{i}g$, where g is a real constant. For several strongly correlated quantum systems that this non-Hermitian generalization is equivalent to multiplying the right hopping energy by e^{g} and the left hopping energy e^{-g}. We demonstrate for these models that we can obtain the correlation length only by observing non-Hermitian energy spectra after the non-Hermitian generalization; the non-Hermitian critical point g_{c} where the energy gap vanishes for the non-Hermitian model is equal to the inverse correlation length of the Hermitian model.

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Contents

Chapter 1

Introduction of a non-Hermitian analysis of strongly correlated quantum systems

In the present thesis, we conjecture for strongly correlated quantum systems that the imaginary part of a zero of the dispersion relation of the elementary excitation in the complex momentum space is equal to the inverse correlation length due to the energy gap of the elementary excitation. The dispersion relation in the complex momentum space is obtained by analytic continuation of the one on the real axis.

For non-interacting systems, the static correlation function $c(x)$, namely, the equal-time one-particle Green's function has the form [1]

$$c(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{4\pi\epsilon(k)} dk, \tag{1.1}$$

where $\epsilon(k)$ denotes the dispersion relation of the elementary excitation at the momentum k. We assume that analytic continuation of $\epsilon(k)$ is valid everywhere in the complex k plane. We define the correlation length ξ corresponding to the excitation as

$$\frac{1}{\xi} \equiv -\lim_{x\to\infty} \frac{\ln|c(x)|}{x}. \tag{1.2}$$

We assume $\left|e^{ikx}/4\pi\epsilon(k)\right| \to 0$ for $|k| \to \infty$ in the upper half-plane in order to make the following discussion easy. By setting the counter of the integration in Eq. (1.1) a semicircle closed on the upper half-plane, the correlation function $c(x)$ is calculated as the summation of the residues of the integrand in Eq. (1.1) at the zeros of $\epsilon(k)$ located in the upper half-plane; specifically, $c(x)$ can have the form

$$c(x) = \sum_{m=1}^{M} A_m e^{ik_m x}, \tag{1.3}$$

where k_m is a zero in the upper half-plane, M is the number of the zeros in the upper half-plane and A_m is a constant. We may consider that $|c(x)|$ behaves for large x as

$$|c(x)| \sim e^{-\kappa x}, \tag{1.4}$$

where κ is the imaginary part of a zero nearest to the real axis in the upper half-plane. We can conclude from Eqs. (1.2) and (1.4) that the imaginary part of a zero nearest to the real axis is equal to the inverse correlation length.

For strongly correlated quantum systems, however, it is not trivial to express the the equal-time one-particle Green's function in the form (1.1). It is one of our conclusions that there may still be a universal relation between the correlation length and the imaginary part of a zero of the dispersion relation of an elementary excitation.

Is the analytic continuation of the dispersion relation valid everywhere in the complex momentum space for strongly correlated systems? We presume that the answer is no; the analytic continuation may be valid only near the real axis in the complex momentum space. In order to determine the area where the analytic continuation of the dispersion relation is valid and to search zeros in this area, we consider a problem of calculating the dispersion relation $\epsilon(p)$ on the axis $\mathrm{Im}\, p = g$, that is, on the axis where the imaginary part of the momentum p is a real constant g. Specifically, we introduce the parameter g which makes the low-energy part of the Hermitian Hamiltonian of the form

$$\mathcal{H} \cong \sum_{-\pi<p<\pi} \epsilon(p)\eta_p^\dagger \eta_p \tag{1.5}$$

transformed to the non-Hermitian one of the form

$$\mathcal{H}(g) \cong \sum_{-\pi<p<\pi} \epsilon(p+\mathrm{i}g)\eta_p^\dagger \eta_p, \tag{1.6}$$

where $\eta_p^\dagger$ and η_p are the creation and annihilation operators of the elementary excitation and $\epsilon(p)$ is the dispersion relation of the elementary excitation.

We reveal for several exactly solved models that obtaining the dispersion relation $\epsilon(p)$ on the axis $\mathrm{Im}\, p = g$ is equivalent to solving non-Hermitian models where an imaginary vector potential $\mathrm{i}\vec{g}$ (where $\vec{g}$ is a real vector) is added to the momentum operator. The non-Hermitian kinetic energy in the continuous space is given by [2]

$$\mathcal{H}_\mathrm{k} = \frac{(-\mathrm{i}\hbar\vec{\nabla} + \mathrm{i}\vec{g})^2}{2m}. \tag{1.7}$$

Its second-quantized form within the tight-binding approximation in the d-dimensional case is given by

$$\mathcal{H}_\mathrm{k} = -t\sum_{\nu=1}^{d}\sum_{\vec{x}} \left(e^{g_\nu(\vec{x})} c_{\vec{x}+\vec{e}_\nu}^\dagger c_{\vec{x}} + e^{-g_\nu(\vec{x})} c_{\vec{x}}^\dagger c_{\vec{x}+\vec{e}_\nu} \right) \tag{1.8}$$

after the Pierels substitution of the imaginary vector potential [2]. We hereafter focus on the one-dimensional case with a constant imaginary vector potential and use

$$\mathcal{H}_\mathrm{k} = -t\sum_{x} (e^{g} c_{x+1}^\dagger c_x + e^{-g} c_x^\dagger c_{x+1}), \tag{1.9}$$

where g is a real constant; in other words, we make the hopping energy asymmetric. More generally, we multiply the right hopping energy $-tc_{x+n}^\dagger c_x$ by e^{ng} and the left hopping energy $-tc_x^\dagger c_{x+n}$ by e^{-ng} in the original Hermitian Hamiltonian. We call the transformation (1.9) a non-Hermitian generalization of quantum systems.

Let us exemplify the above on the half-filled Hubbard model. Obtaining the dispersion relation $\epsilon(p)$ of the charge excitation on the axis $\mathrm{Im}\, p = g$ may be actually equivalent to solving the non-Hermitian model [3]

$$\mathcal{H}_{\mathrm{Hubbard}}(g) = -t\sum_{l=1}^{L}\sum_{\sigma=\uparrow,\downarrow}(e^{g}c_{l+1,\sigma}^\dagger c_{l,\sigma} + e^{-g}c_{l,\sigma}^\dagger c_{l+1,\sigma}) + U\sum_{l=1}^{L} n_{l,\uparrow}n_{l,\downarrow}, \tag{1.10}$$

which was first introduced by Fukui and Kawakami. They solved analytically the non-Hermitian Hubbard model (1.10) in the thermodynamic limit by the Bethe-ansatz method. They argued that the "Hubbard gap" vanishes at $g = g_{\mathrm{c}}$ as we increase the non-Hermiticity g and obtained an analytical expression of the non-Hermitian critical point g_{c}. We pointed out [4] that the non-Hermitian critical point g_{c} is actually equal to the inverse correlation length of the charge excitation. This equality may be understood quite naturally by considering that the imaginary part of a zero of the dispersion relation of the charge excitation is equal to the inverse correlation length and that the Hamiltonian (1.10) yields the dispersion relation $\epsilon(p)$ of the charge excitation on the axis $\mathrm{Im}\, p = g$.

It is remarkable that we can obtain the length scale, namely, the correlation length due to the energy gap only by observing the behavior of the non-Hermitian spectrum. It is a purpose of the non-Hermitian generalization that we can obtain the length scale of Hermitian quantum systems only from non-Hermitian energy spectra. The non-Hermitian generalization in Eqs. (1.7)-(1.9) was first introduced and applied to the one-electron Anderson model in a random potential by Hatano and Nelson [2]. Their model is, in one dimension,

$$\mathcal{H}_{\mathrm{random}}(g) = -t\sum_{x=1}^{L}\left(e^{g}|x+1\rangle\langle x| + e^{-g}|x\rangle\langle x+1|\right) + \sum_{x=1}^{L} V_x|x\rangle\langle x|, \tag{1.11}$$

where V_x is a random potential at site x and we require the periodic boundary condition. As we increase the non-Hermiticity g, a pair of neighboring eigenvalues collide at a point $g = g_{\mathrm{c}}$ and then become complex [5]. It was revealed [2] that the non-Hermitian critical point g_{c} is equal to the inverse localization length of the eigenfunction of the original Hermitian Hamiltonian; see Appendix A. The non-Hermitian energy spectra of the systems *with* randomness and *without* interactions thus yield the localization length. In the present thesis, we try to claim that the non-Hermitian spectra of the systems *without* randomness and *with* interactions yield the correlation length.

The present thesis is organized as follows; we discuss the $S = 1/2$ ferromagnetic isotropic XY chain in a magnetic field in Chapter 2, the half-filled Hubbard model in Chapter 3 and the $S = 1/2$ XXZ chain in the Ising-like region in Chapter 4. For these models, we first point out that the imaginary part of a zero of the dispersion relation is equal to the inverse or twice the inverse correlation length. The factor one or two corresponds to the number of the elementary excitations involved in the excited state. We next use non-Hermitian models in order to calculate the dispersion relation on the axis $\mathrm{Im}\, p = g$ with a real constant g. By analyzing the non-Hermitian models, we argue that the non-Hermitian critical point g_c where the energy gap vanishes is equal to the inverse correlation length. It supports our conjecture proposed at the beginning of the introduction. We numerically determine the area in the complex momentum space where the analytic continuation of the Hermitian dispersion relation is valid. We search zeros in the area analytically for the $S = 1/2$ ferromagnetic isotropic XY chain in a magnetic field and numerically for the half-filled Hubbard model and for the $S = 1/2$ XXZ chain in the Ising-like region. We argue that the zeros nearest to the real axis in this area correspond to the non-Hermitian critical point g_c.

We have a prospect that the non-Hermitian generalization in Eq. (1.9) is also applicable to unsolved systems. In Chapter 5, we analyze the Majumdar-Ghosh model, for which we do not know the energy gap exactly; only approximate estimates are known. We still show that the non-Hermitian critical point g_c, where approximate estimates of the energy gap vanish, is equal to the inverse correlation length calculated, by finite-size scaling of the correlation function of the ground state of the Hermitian Majumdar-Ghosh model.

In Chapter 6, we numerically analyze non-Hermitian models of finite size L. We calculate the non-Hermitian "critical" point $g_c(L)$ where the energy of the eigenstate corresponding to the ground state in the limit $L \to \infty$ becomes complex; we then obtain an extrapolated estimate $g_c(\infty)$. We numerically confirm that the estimate $g_c(\infty)$ and the inverse correlation length of the Hermitian systems are consistent for the Hubbard model and for the $S = 1/2$ XXZ chain. We also analyze an unsolved model, namely the $S = 1/2$ antiferromagnetic Heisenberg chain with nearest- and next-nearest-neighbor interactions including the Majumdar-Ghosh model.

In the summary, we conjecture again for strongly correlated quantum systems that it may be a universal relation that the imaginary part of a zero of the dispersion relation is equal to the inverse correlation length. We next give some examples for which the non-Hermitian generalization in Eq. (1.9) does not work well in order to obtain the correlation length. However, our conjecture proposed at the beginning of the introduction is valid ever for these examples.

Chapter 2

$S = 1/2$ isotropic XY chain

2.1 Zeros of the dispersion relation of the elementary excitation and the correlation length

We first consider as an introductory example the $S = 1/2$ ferromagnetic isotropic XY chain in a magnetic field which is mapped to a non-interacting Fermion system. The Hamiltonian of this model is

$$\mathcal{H}_{XY} = -J \sum_{l=1}^{L} \left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y \right) - h \sum_{l=1}^{L} S_l^z, \tag{2.1}$$

where we set $J > 0$. The Hamiltonian (2.1) is transformed into

$$\mathcal{H}_{XY} = -\frac{J}{2} \sum_{l=1}^{L} (c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1}) - \frac{hL}{2} + h \sum_{l=1}^{L} c_l^\dagger c_l \tag{2.2}$$

by the Jordan-Wigner transformation

$$c_j = 2^{j-1} S_1^z S_2^z \dots S_{j-1}^z S_j^+, \qquad c_j^\dagger = 2^{j-1} S_1^z S_2^z \dots S_{j-1}^z S_j^-. \tag{2.3}$$

We can immediately diagonalize the Hamiltonian (2.2) in the form

$$\mathcal{H}_{XY} = \sum_{-\pi < p < \pi} \epsilon(p) c_p^\dagger c_p - \frac{hL}{2} \tag{2.4}$$

with the Fourier transformation

$$c_p = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{-\mathrm{i}pl} c_l, \quad c_p^\dagger = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{\mathrm{i}pl} c_l^\dagger, \tag{2.5}$$

where $\epsilon(p) \equiv -J \cos p + h$ is the dispersion relation of the one-particle excitation shown in Fig. 2.1 for $h > J$. The ground state for $h > J$ has no Fermions and its the eigenenergy is $-hL/2$. The first excited state is the one-particle excitation of the momentum $p = 0$ and its excitation energy is $h - J$.

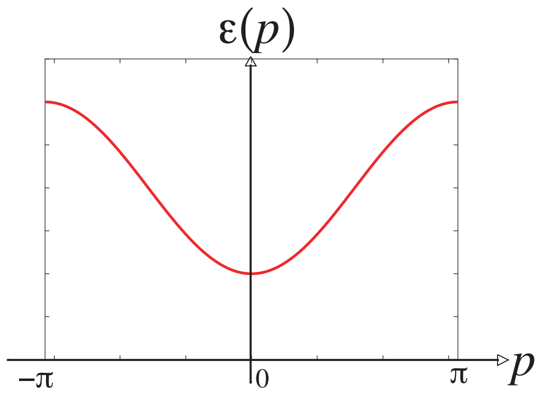


Figure 2.1: The dispersion relation $\epsilon(k) = h - J\cos p$ of the one-particle excitation for the $S = 1/2$ isotropic XY chain for $h > J$.

Let us obtain the zero $p^{(0)}$ of the dispersion relation $\epsilon(p)$ of the one-particle excitation in the complex momentum space. The equation

$$h - J\cos(p_r^{(0)} + ip_i^{(0)}) = 0 \tag{2.6}$$

yields the equation for the real $p_r^{(0)} \equiv \mathrm{Re}\, p^{(0)}$ part of the form

$$h - J\cos p_r^{(0)} \cosh p_i^{(0)} = 0 \tag{2.7}$$

and the one for the imaginary part $p_i^{(0)} \equiv \mathrm{Im}\, p^{(0)}$ of the form

$$\sin p_r^{(0)} \sinh p_i^{(0)} = 0. \tag{2.8}$$

By solving Eqs. (2.7) and (2.8), we obtain the zero $p^{(0)}$ in the region $\mathrm{Im}\, p \geq 0$ of the form

$$p^{(0)} = \mathrm{i}\ln\left[\frac{h}{J} + \sqrt{\left(\frac{h}{J}\right)^2 - 1}\right]; \tag{2.9}$$

its imaginary part is equal to the inverse correlation length obtained by the quantum transfer matrix method [6].

We hereafter briefly review the calculation of the correlation length $\xi(T)$ at finite temperature T by the quantum transfer matrix method. The eigenvalues of the quantum transfer matrix yields the correlation length $\xi(T)$ of the form

$$\frac{1}{\xi} = \lim_{N_\mathrm{T}\to\infty}\left|\frac{\Lambda_{N_\mathrm{T}}^{(\mathrm{Max})}}{\Lambda_{N_\mathrm{T}-1}^{(\mathrm{Max})}}\right|, \tag{2.10}$$

where $\Lambda_{N_\mathrm{T}}^{(\mathrm{Max})}$ is the largest eigenvalue in the subspace where the Trotter number, that is, the number of slices along the imaginary time axis, is N_T. For the isotropic XY chain, the eigenvalues $\lim_{N_\mathrm{T}\to\infty}\Lambda_{N_\mathrm{T}}^{(\mathrm{Max})}$ and $\lim_{N_\mathrm{T}\to\infty}\Lambda_{N_\mathrm{T}-1}^{(\mathrm{Max})}$ at finite temperature T

are obtained in the forms [7]

$$\lim_{N_{\mathrm{T}}\to\infty} \Lambda_{N_{\mathrm{T}}}^{(\mathrm{Max})} = \exp\left[\frac{1}{2\pi}\int_0^{2\pi} dp \ln\left(2\cosh\left(\frac{J\cos p + h}{2T}\right)\right)\right], \tag{2.11}$$

$$\lim_{N_{\mathrm{T}}\to\infty} \Lambda_{N_{\mathrm{T}}-1}^{(\mathrm{Max})} = \frac{J}{2T}\exp\left[\frac{1}{2\pi}\int_0^{2\pi} dp \ln\left(\frac{\sinh[(J\cos p + h)/2T]}{(J\cos p + h)/2T}\right)\right]. \tag{2.12}$$

By substituting Eq. (2.12) into Eq. (2.10), we have the correlation length $\xi(T)$ at finite temperature T of the form

$$\frac{1}{\xi(T)} = \ln\left[\frac{h}{J} + \sqrt{\left(\frac{h}{J}\right)^2 - 1}\right] + \frac{1}{2\pi}\int_0^{2\pi} dp \ln\left[2\coth\left(\frac{J\cos p + h}{2T}\right)\right]. \tag{2.13}$$

By taking the limit $T \to 0$, we can neglect the second term of the right hand-side in Eq. (2.13) and we thus have the inverse correlation length $1/\xi(0)$ of the form

$$\frac{1}{\xi(0)} = \ln\left[\frac{h}{J} + \sqrt{\left(\frac{h}{J}\right)^2 - 1}\right], \tag{2.14}$$

which is equal to the imaginary part of the zero (2.9).

2.2 Non-Hermitian analysis of the isotropic *XY* chain

We propose a non-Hermitian isotropic XY chain in order to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$ and discuss the spectral behavior of the non-Hermitian model.

Let us transform the Hermitian Hamiltonian (2.4) to the non-Hermitian one of the form

$$\mathcal{H}_{XY}(g) = \sum_{-\pi<p<\pi} \epsilon(p + \mathrm{i}g) c_p^\dagger c_p - \frac{hL}{2} \tag{2.15}$$

as we described in Eq. (1.6), in order to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$. In the real space, the non-Hermitian Hamiltonian (2.15) becomes

$$\mathcal{H}_{XY}(g) = -\frac{J}{2}\sum_{l=1}^{L}(e^g c_{l+1}^\dagger c_l + e^{-g} c_l^\dagger c_{l+1}) - \frac{hL}{2} + h\sum_{l=1}^{L} c_l^\dagger c_l. \tag{2.16}$$

The expression (2.16) actually corresponds to the non-Hermitian generalization in Eq. (1.9). By the inverse Jordan-Wigner transformation, the Hamiltonian (2.16) is transformed back into

$$\begin{aligned}\mathcal{H}_{XY}(g) =& -\frac{J}{2}\sum_{l=1}^{L}\left[e^g S_l^- S_{l+1}^+ + e^{-g} S_l^+ S_{l+1}^-\right] - h\sum_{l=1}^{L} S_l^z \\ =& -J\sum_{l=1}^{L}\left[\cosh g\left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y\right) + \mathrm{i}\sinh g\left(S_l^y S_{l+1}^x + S_l^x S_{l+1}^y\right)\right] - h\sum_{l=1}^{L} S_l^z.\end{aligned} \tag{2.17}$$

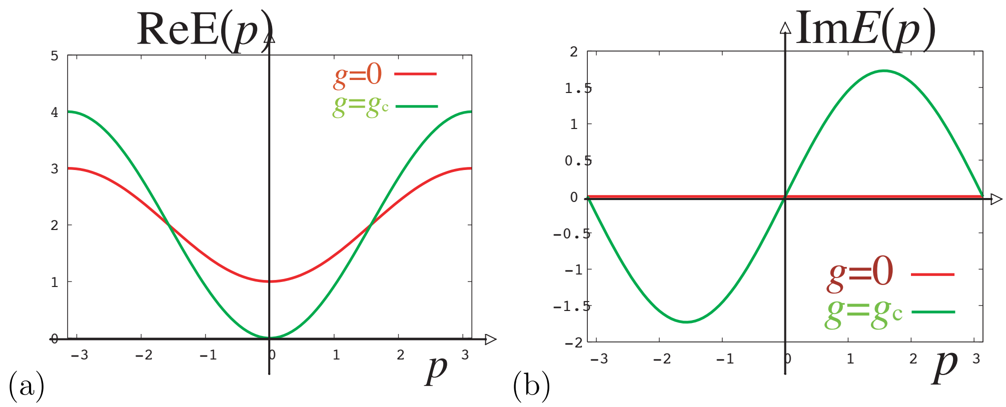


Figure 2.2: (a) The real part of $\mathcal{E}(p)$ and (b) the imaginary part of $\mathcal{E}(p)$ for $h > J$, where g_c denotes the non-Hermitian critical point defined in Eq. (2.20).

We obtain the ground-state energy and the excitation energy by the one-particle excitation. The ground state has no Fermions and its eigenenergy is $E_\mathrm{gs} = -hL/2$, which does not depend on g. On the other hand, the one-particle excitation energy $\mathcal{E}(p)$ at the momentum p is

$$\mathcal{E}(p) = \epsilon(p + ig) = -J\cos(p + ig) + h, \tag{2.18}$$

whose real part $\mathrm{Re}\,\mathcal{E}(p)$ and imaginary part $\mathrm{Im}\,\mathcal{E}(p)$ are schematically shown in Fig. 2.2. Figure 2.3 shows the energy spectra of the non-Hermitian XY chain (2.16) for $h > J$. The symbol $\times$ denotes the ground state and the solid lines denote the one-particle excitations. All eigenvalues are real at the Hermitian point $g = 0$ and $\epsilon(0) = h - J$ gives the finite energy gap as shown in Fig. 2.3 (a). As we turn on the non-Hermiticity g, all eigenvalues except for $p = 0$ and $\pm\pi$ immediately spread into the complex E plane (Fig. 2.3 (b)). The g dependence of the energy gap $\Delta E(g)$ is

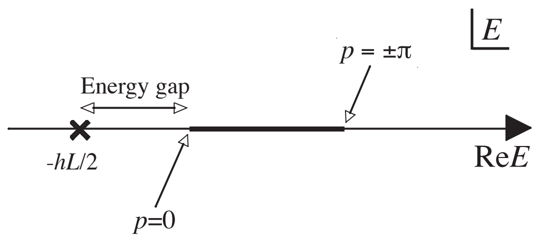
$$\Delta E(g) = \epsilon(ig) = h - J\cosh g. \tag{2.19}$$

We define the non-Hermitian critical point g_c as the point where the energy gap above the ground state vanishes. From Eq. (2.19), we obtain the non-Hermitian critical point g_c of the form

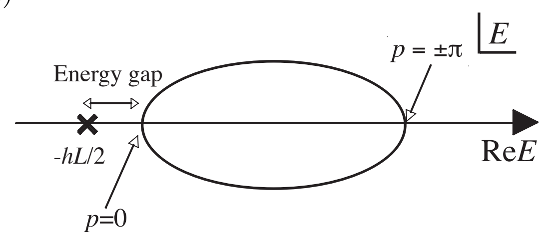
$$g_\mathrm{c} = \ln\left[\frac{h}{J} + \sqrt{\left(\frac{h}{J}\right)^2 - 1}\right]. \tag{2.20}$$

Figure 2.4 shows the non-Hermitian critical point g_c as a function of h/J. The Hermitian system is gapless (the XY phase) for $h < J$ and hence we have the non-Hermitian critical point $g_\mathrm{c} = 0$ in the region. We can immediately confirm that the analytical expression of the non-Hermitian critical point g_c in Eq. (2.20) is equal to the inverse correlation length of the Hermitian system [6].

Indeed, to see where the gap (2.19) vanishes is equivalent to solve Eq. (2.7). This is how the non-Hermitian generalization of the form (1.9) may give a zero



(a)



(b)

Figure 2.3: The eigenvalue distributions of the non-Hermitian isotropic XY chain for $h > J$ for (a) $g = 0$ and (b) $0 < g < g_c$. The symbol $\times$ denotes the ground state.

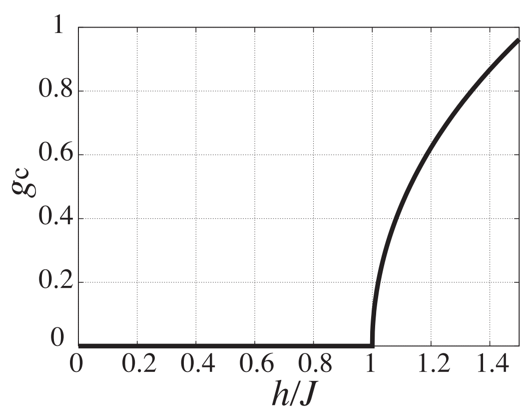


Figure 2.4: The non-Hermitian critical point g_c of the isotropic XY chain. The ground-state critical point of the Hermitian system is $h/J = 1$.

of the dispersion relation and hence give the inverse correlation length. In the region $g \geq g_c$, the ground-state energy energy E_{gs} denoted by $\times$ in Fig. (2.3) does not become complex because the ground state is in a different subspace from any excited states. This behavior is quite different from the one for the non-Hermitian Hubbard model (3.11) and for the non-Hermitian $S = 1/2$ antiferromagnetic XXZ chain (4.15) as shown below.

2.3 Non-Hermitian analysis of the $S = 1/2$ transverse Ising chain

We here comment that the non-Hermitian generalization of the form Eq. (1.9), that is, multiplying the right hopping energy e^g and the left hopping energy by e^{-g} in the Hermitian Hamiltonian, does not work for the $S = 1/2$ ferromagnetic transverse Ising chain

$$\mathcal{H}_{\text{Ising}} = -J \sum_{l=1}^{L} S_l^x S_{l+1}^x - h \sum_{l=1}^{L} S_l^z \tag{2.21}$$

in order to obtain the correlation length. Our conjecture is nevertheless supported for this model; the imaginary part of a zero of the dispersion relation is equal to the inverse correlation length.

First, let us obtain the zeros of the dispersion relation of the Hermitian model. The Hamiltonian (2.21) is transformed into

$$\mathcal{H}_{\text{Ising}} = -\frac{J}{4} \sum_{l=1}^{L} (c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l^\dagger - c_l c_{l+1}) - \frac{hL}{2} + h \sum_{l=1}^{L} c_l^\dagger c_l \tag{2.22}$$

by the Jordan-Wigner transformation in Eq. (2.3). By the Fourier transformation of the Fermionic operators $c_l^\dagger$ and c_l,

$$c_k = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{-ikl} e^{-\frac{\pi}{4}i} c_l, \qquad c_k^\dagger = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{ikl} e^{\frac{\pi}{4}i} c_l^\dagger, \tag{2.23}$$

the Hamiltonian (2.22) is rewritten in the form

$$\mathcal{H}_{\text{Ising}} = -\frac{hL}{2} - \sum_{0<k<\pi} \left[(\frac{J}{2}\cos k - h)(c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) + \frac{J}{2}\sin k (c_k^\dagger c_{-k}^\dagger + c_{-k} c_k) \right]. \tag{2.24}$$

The elementary excitation of Eq. (2.24) is given by

$$\begin{aligned} \eta_p &= \cos\theta_p c_p - \sin\theta_p c_{-p}^\dagger, \\ \eta_{-p} &= \sin\theta_p c_p^\dagger + \cos\theta_p c_{-p}, \end{aligned} \tag{2.25}$$

where

$$\theta_p = -\frac{1}{2} \arctan\left[\frac{J \sin p}{J \cos p - 2h} \right]. \tag{2.26}$$

The Hamiltonian (2.21) is therefore diagonalized in the momentum space of the form

$$\mathcal{H}_{\text{Ising}} = \sum_{-\pi<p<\pi} \epsilon(p) \left(\eta_p^\dagger \eta_p - \frac{1}{2} \right), \tag{2.27}$$

where the dispersion relation $\epsilon(p)$ is given by

$$\epsilon(p) = \sqrt{\left(\frac{J\cos p}{2} - h \right)^2 + \left(\frac{J\sin p}{2} \right)^2}. \tag{2.28}$$

We then obtain zeros $p^{(0)}$ of the dispersion relation (2.28). By introducing $p_r^{(0)} \equiv \operatorname{Re} p^{(0)}$ and $p_i^{(0)} \equiv \operatorname{Im} p^{(0)}$, the equation

$$\left(\frac{J\cos(p_r^{(0)} + ip_i^{(0)})}{2} - h \right)^2 + \left(\frac{J\sin(p_r^{(0)} + ip_i^{(0)})}{2} \right)^2 = 0 \tag{2.29}$$

yields the equation for the real part of the form

$$\frac{J^2}{4} + h^2 - Jh\cos p_r^{(0)} \cosh p_i^{(0)} = 0 \tag{2.30}$$

and the one for the imaginary part of the form

$$\sin p_r^{(0)} \sinh p_i^{(0)} = 0. \tag{2.31}$$

By solving Eqs. (2.30) and (2.31), we obtain the zeros $p^{(0)}$ of the dispersion relation (2.28) in the region $\operatorname{Im} p \geq 0$ of the form

$$p^{(0)} = \mathrm{i} \left| \ln \left(\frac{2h}{J} \right) \right|. \tag{2.32}$$

The imaginary part of the zeros (2.32) is equal to the inverse correlation length of the transverse Ising chain. The correlation length is obtained from asymptotic form of the two-point correlation function $\langle S_l^x S_{l+n}^x \rangle$, which is given for large n in the form [8]

$$\begin{aligned} &\langle S_l^x S_{l+n}^x \rangle \\ &\simeq \frac{1}{4} \left(1 - \left(\frac{2h}{J} \right)^2 \right) \pi^{-1/2} n^{-1/2} \left(\frac{2h}{J} \right)^{-n} \left[1 - \frac{1}{8} n^{-1} \left(1 + \left(\frac{2h}{J} \right)^2 \right) \left(1 - \left(\frac{2h}{J} \right)^{-1} \right) + O(n^{-2}) \right] \\ &\simeq \exp(-n/\xi). \end{aligned} \tag{2.33}$$

with the inverse correlation length $1/\xi = \ln(2h/J)$.

Next, we derive a non-Hermitian Hamiltonian of the form (1.6) by replacing p with $p + \mathrm{i}g$ in the dispersion relation $\epsilon(p)$ in order to obtain the dispersion relation on the axis $\operatorname{Im} p = g$. As shown in Appendix B, the Hamiltonian is transformed back to the spin Hamiltonian of the form

$$\begin{aligned} &\mathcal{H}_{\text{Ising}}(g) \\ &= \sum_l \sum_{n=1}^{\infty} (-2)^n S_{l+1}^z \dots S_{l+n-1}^z \left[(\alpha_n - \gamma_n) S_{l+n}^x S_l^x + (\alpha_n + \gamma_n) S_{l+n}^y S_l^y + \mathrm{i}\beta_n (S_{l+n}^x S_l^y - S_{l+n}^y S_l^x) \right] \\ &\quad - \alpha_0 \sum_l S_l^z, \end{aligned} \tag{2.34}$$

where coefficients α_n, β_n and γ_n are given by the following integrals:

$$
\begin{aligned}
\alpha_n &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{J\cos p}{2} - h\right)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}\cos(np)\mathrm{d}p, \\
\beta_n &= \frac{\mathrm{i}}{2\pi}\int_{-\pi}^{\pi}\frac{\epsilon(p+\mathrm{i}g)-\epsilon(p-\mathrm{i}g)}{2}\sin(np)\mathrm{d}p, \\
\gamma_n &= -\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{J\sin p}{2}\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}\sin(np)\mathrm{d}p.
\end{aligned}
\tag{2.35}
$$

This non-Hermitian Hamiltonian is very complicated; interactions between spins beyond the nearest neighbor sites emerge as soon as g is finite. It is because its elementary excitation is obtained by the Bogoliubov transformation; the creation and annihilation operators at two different momenta p and $-p$ are mixed. Conversely, the non-Hermitian generalization of the simple form (1.9) does not produce the dispersion relation $\epsilon(p+\mathrm{i}g)$ in this model. We may need another principle of a non-Hermitian generalization for this model.

Chapter 3

Half-filled Hubbard model

In the present chapter, we consider the half-filled Hubbard model

$$\mathcal{H}_{\text{Hubbard}} = -t \sum_{l=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (c_{l+1,\sigma}^{\dagger} c_{l,\sigma} + c_{l,\sigma}^{\dagger} c_{l+1,\sigma}) + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}. \tag{3.1}$$

The charge excitation has a finite energy gap, namely, the Hubbard gap for $U > 0$. By considering the finite-size scaling of the Drude weight, Stafford and Millis obtained the inverse correlation length of the charge excitation of the form [9]

$$\frac{1}{\xi} = \text{arcsinh}(U/4t) - 2 \int_{0}^{\infty} \frac{J_0(\omega)\sinh(\omega U/4t)}{\omega(1+e^{\omega U/2t})} \mathrm{d}\omega, \tag{3.2}$$

where $J_0(\omega)$ is the Bessel function of the first kind. The Drude weight is defined as [10]

$$D \equiv \frac{1}{2} \frac{d^2 E_0}{d^2 \phi} \bigg|_{\phi=0} \tag{3.3}$$

for the Hubbard chain under the magnetic field, whose Hamiltonian is given by

$$\mathcal{H} = -t \sum_{l=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{i\phi} c_{l+1,\sigma}^{\dagger} c_{l,\sigma} + e^{-i\phi} c_{l,\sigma}^{\dagger} c_{l+1,\sigma}) + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}, \tag{3.4}$$

where ϕ is a real constant and E_0 is the ground-state energy per site. They solved the Hamiltonian (3.4) in the half-filled case for large enough size L by the Bethe-ansatz method and asymptotically obtained the L dependence of the ground state energy $E_0(L)$. By applying Eq. (3.3), they obtained the expression (3.2) from the L dependence of the Drude weight $D(L)$ of the form [9]

$$D(L) = (-1)^{L/2+1} L^{1/2} F(U/t) e^{-L/\xi} \tag{3.5}$$

for large L, where $F(U/t)$ is a U-dependent function given by

$$F(U/t) \equiv \frac{\left(\frac{U}{4t}\right)^2 - \sqrt{1+\left(\frac{U}{4t}\right)^2} \int_0^{\infty} dx\, e^{-x} \tanh(x) J_1(4tx/U)}{\sqrt{\frac{\pi}{2} \int_0^{\infty} dx\, e^{-x} J_0(4tx/U) \left[\left(\frac{U}{4t}\right)^2 + \left(1+\left(\frac{U}{4t}\right)^2\right) x \tanh(x)\right]}}. \tag{3.6}$$

3.1 Zeros of the dispersion relation of the charge excitation and the correlation length

We first point out for the half-filled Hubbard model that the imaginary part of a zero of the dispersion relation of the charge excitation is equal to the inverse correlation length of the half-filled Hubbard model given in Eq. (3.2).

We obtain the dispersion relation in the complex momentum space by considering the analytic continuation of the Hermitian dispersion, which has been already known; specifically, the charge excitation of the half-filled Hubbard model has the excitation energy $\mathcal{E}(k_h)$ of the form [11]

$$\mathcal{E}(k_h) = U + 4t\cos k_h + 8t\int_0^\infty \frac{\cos(\omega\sin k_h)J_1(\omega)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega \tag{3.7}$$

and the momentum $p(k_h)$ of the form

$$p(k_h) = k_h + 2\int_0^\infty \frac{\sin(\omega\sin k_h)J_0(\omega)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega, \tag{3.8}$$

where k_h is the quasimomentum of the "hole". The dispersion relation of the charge excitation $\mathcal{E}(p)$ is thus obtained through the parameter k_h. Fukui and Kawakami obtained zeros $k_h^{(0)}$ of the excitation energy (3.7) on the axis $\mathrm{Re}\,k_h = \pm\pi$ in the *quasimomentum* space in the region $\mathrm{Im}\,k_h \geq 0$ of the form [3]

$$k_h^{(0)} = \pm\pi + \mathrm{i}\ \mathrm{arcsinh}(U/4t). \tag{3.9}$$

By substituting Eq. (3.9) into Eq. (3.8), we have the corresponding zeros $p_h^{(0)}$ of the dispersion relation in the *momentum* space in the region $\mathrm{Im}\,p_h \geq 0$ as

$$p_h^{(0)} = \pm\pi + \mathrm{i}\left[\mathrm{arcsinh}(U/4t) - 2\int_0^\infty \frac{J_0(\omega)\sinh(\omega U/4t)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega\right]. \tag{3.10}$$

The imaginary part of zeros $p_h^{(0)}$ is equal to the inverse correlation length of the charge excitation in Eq. (3.2). Figure 3.1 shows numerical calculation of the real part of the excitation energy $\mathcal{E}(p)$ in the complex momentum space in the region $\mathrm{Im}\,p \leq 1/\xi$ for $U/t = 4$; it suggests that the zeros in Eq. (3.10) are the nearest to the real axis.

In the next section, we use a non-Hermitian Hubbard model for the purpose of obtaining the dispersion relation on the axis $\mathrm{Im}\,p = g$. We then argue where the analytic continuation of the dispersion relation may be valid in the complex momentum space. We also conclude that the zeros in Eq. (3.10) actually exist in the area where the analytic continuation is assumed to be valid.

3.2 Non-Hermitian analysis of the Hubbard model

For the purpose of searching zeros in the complex momentum space, we use a non-Hermitian Hubbard model in order to obtaining the dispersion relation on the axis

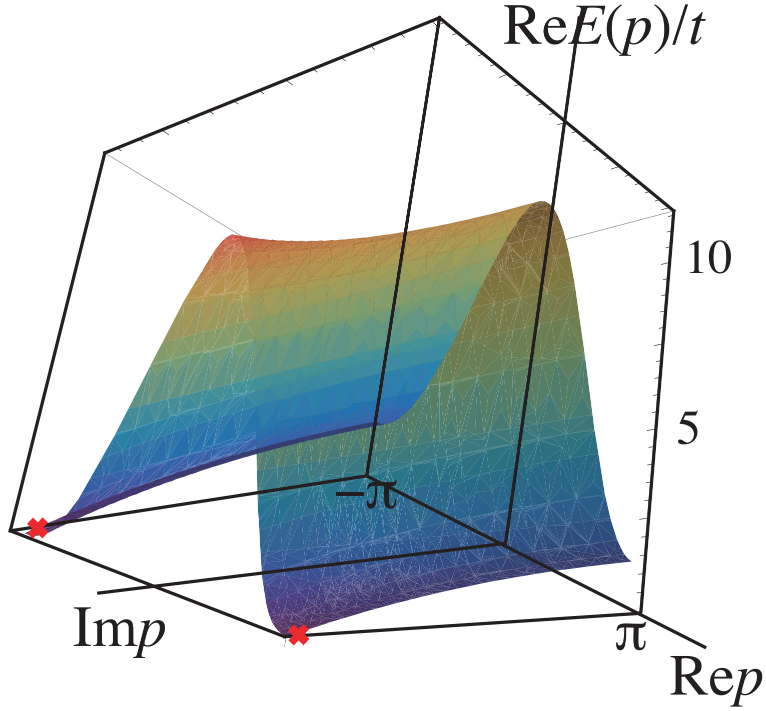


Figure 3.1: The real part of the excitation energy $\mathcal{E}(p)$ in the complex momentum space for $U/t = 4$. The red symbols $\times$ denote the zeros of $\mathcal{E}(p)$, whose imaginary part is $1/\xi$.

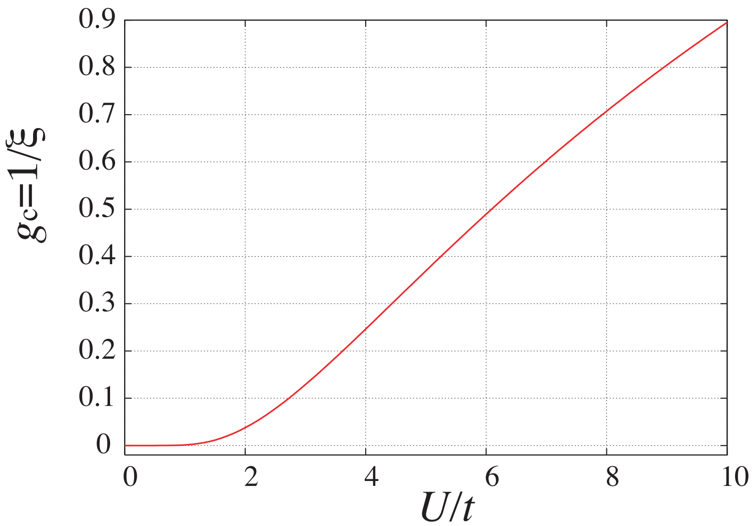


Figure 3.2: The U/t dependence of $g_{\mathrm{c}} = \xi^{-1}$.

$\mathrm{Im}\, p = g$ with real g. As will be demonstrated in §3.2.2, obtaining the dispersion relation on the axis $\mathrm{Im}\, p = g$ may be actually equivalent to solving a non-Hermitian Hubbard model

$$\mathcal{H}_{\mathrm{Hubbard}}(g) = -t \sum_{l=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{g} c_{l+1,\sigma}^{\dagger} c_{l,\sigma} + e^{-g} c_{l,\sigma}^{\dagger} c_{l+1,\sigma}) + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}, \tag{3.11}$$

which was first proposed by Fukui and Kawakami [3]. They solved the non-Hermitian model (3.11) in the half-filled case exactly by the Bethe-ansatz method. They also derived an analytical expression of the non-Hermitian critical point g_{c} where the Hubbard gap vanishes of the form

$$g_{\mathrm{c}} = \mathrm{arcsinh}(U/4t) + 2\mathrm{i} \int_{-\infty}^{\infty} \arctan \frac{\lambda + \mathrm{i}U/4t}{U/4t} \sigma(\lambda) \mathrm{d}\lambda, \tag{3.12}$$

where the distribution function $\sigma(\lambda)$ of the spin rapidity λ is given by

$$\sigma(\lambda) = \frac{1}{2\pi} \int_{0}^{\infty} \mathrm{sech} \left(\frac{\omega U}{4t} \right) \cos(\lambda\omega) J_0(\omega) \mathrm{d}\omega. \tag{3.13}$$

After some algebra in Appendix C, we can show that the analytical expression of the non-Hermitian critical point g_{c} is actually equal to the inverse correlation length $1/\xi$ due to the charge excitation in Eq. (3.2). Figure 3.2 shows the U/t dependence of $g_{\mathrm{c}}(= 1/\xi)$. For large U, we have $g_{\mathrm{c}} \sim \mathrm{arcsinh}(U/4t)$ by neglecting the second term of Eq. (3.2).

We also discuss partly numerically where in the complex momentum space the analytical continuation may be valid by analyzing the non-Hermitian Hubbard model (3.11). We then show that the zeros $p_h^{(0)}$ in Eq. (3.10) actually exist in the area where the analytic continuation of the dispersion relation of the charge excitation is considered to be valid.

In §3.2.1, we review the analytic solution [3] of the non-Hermitian Hamiltonian (3.11) by the Bethe-ansatz method. In §3.2.2, we argue physical meaning of the non-Hermitian generalization of the Hubbard model; the non-Hermiticity g makes the dispersion relation $\mathcal{E}(p)$ of the charge excitation transformed to $\mathcal{E}(p+ig)$.

3.2.1 Exact solution of the non-Hermitian Hubbard model

Bethe-ansatz equation and its exact solution

In order to solve the Hamiltonian (3.11), we make the following ansatz for the right eigenfunction $\Psi_g^{(\mathrm{R})}$, considering the imaginary gauge transformation (A.4) [3]:

$$\begin{aligned}\Psi_g^{(\mathrm{R})}(x_1,\cdots,x_N;\sigma_1,\cdots,\sigma_N) &= \exp\left(g\sum_{j=1}^{N}x_j\right)\Psi_0(x_1,\cdots,x_N;\sigma_1,\cdots,\sigma_N)\\ &= \sum_{\{P\}}\mathrm{sgn}(PQ)A_{\sigma_{Q_1},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_N})\exp(\mathrm{i}\sum_{j=1}^{N}(k_{P_j}-\mathrm{i}g)x_{Q_j}). \end{aligned} \tag{3.14}$$

The wave function Ψ_0 is the Bethe-ansatz wave function in the Hermitian case $g=0$,

$$\Psi_0(x_1,\cdots,x_N;\sigma_1,\cdots,\sigma_N) = \sum_{\{P\}}\mathrm{sgn}(PQ)A_{\sigma_{Q_1},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_N})\exp(\mathrm{i}\sum_{j=1}^{N}k_{P_j}x_{Q_j}), \tag{3.15}$$

where L, M and N are the number of sites, the number of the down spins and the number of the electrons, respectively. The symbols $P=(P_1,P_2,\cdots,P_N)$ and $Q=(Q_1,Q_2,\cdots,Q_N)$ denote permutations of the set $(1,2,\cdots,N)$ with $1\le x_{Q_1}\le x_{Q_2}\le\cdots\le x_{Q_N}\le L$. The symbol $A_{\sigma_{Q_1},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_N})$ is a set of $N!\times N!$ coefficients depending on the two permutations P and Q. The quasimomenta $k_1,k_2,\cdots,k_N$ are unequal to each other for the ground state [12].

The non-Hermitian Bethe-ansatz equation is then given by [3] (see Appendix D)

$$\begin{aligned}\exp(\mathrm{i}Lk_j+gL) &= \prod_{\beta=1}^{M}\frac{\sin k_j-\lambda_\beta+\mathrm{i}U/4t}{\sin k_j-\lambda_\beta-\mathrm{i}U/4t} \qquad (j=1,\cdots,N),\\ \prod_{j=1}^{N}\frac{\sin k_j-\lambda_\alpha+\mathrm{i}U/4t}{\sin k_j-\lambda_\alpha-\mathrm{i}U/4t} &= -\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta-\mathrm{i}U/2t}{\lambda_\alpha-\lambda_\beta+\mathrm{i}U/2t} \qquad (\alpha=1,\cdots,M).\end{aligned} \tag{3.16}$$

By taking the logarithm of Eq. (3.16), we have

$$k_jL-\mathrm{i}gL = 2\pi I_j - 2\sum_{\beta=1}^{M}\arctan\frac{\sin k_j-\lambda_\beta}{U/4t} \qquad (j=1,\cdots,N), \tag{3.17}$$

$$-2\sum_{j=1}^{N}\arctan\frac{\sin k_j-\lambda_\alpha}{U/4t} = 2\pi J_\alpha + 2\sum_{\beta=1}^{M}\arctan\frac{\lambda_\alpha-\lambda_\beta}{U/2t} \qquad (\alpha=1,\cdots,M), \tag{3.18}$$

where we set the quantum numbers I_j and J_α of the ground state for even N and odd M as follows [13]:

$$I_j = \frac{N-1}{2}, \frac{N-3}{2}, \cdots, -\frac{N-1}{2}, \tag{3.19}$$

$$J_\alpha = \frac{M-1}{2}, \frac{M-3}{2}, \cdots, -\frac{M-1}{2}. \tag{3.20}$$

We here consider the half-filled case where $L = N$ and $M = N/2$. By taking the thermodynamic limit $L \to \infty$ of Eqs. (3.17) and (3.18), we obtain the Fredholm-type integral equations:

$$k - \mathrm{i}g = 2\pi z_{\mathcal{C}}(k) - \int_{\mathcal{S}(g)} 2\arctan\frac{\sin k - \lambda}{U/4t}\sigma(\lambda)d\lambda \qquad \text{for } k \in \mathcal{C}(g), \tag{3.21}$$

$$\int_{\mathcal{C}(g)} 2\arctan\frac{\lambda - \sin k}{U/4t}\rho(k)dk = 2\pi z_{\mathcal{S}}(\lambda) + \int_{\mathcal{S}(g)} 2\arctan\frac{\lambda-\lambda'}{U/2t}\sigma(\lambda')d\lambda' \qquad \text{for } \lambda \in \mathcal{S}(g). \tag{3.22}$$

In Eqs. (3.21) and (3.22), we introduced functions $z_{\mathcal{C}}(k)$ and $z_{\mathcal{S}}(\lambda)$ by taking the continuous limit $L \to \infty$ of the discrete functions $z_{\mathcal{C}}(k_j) \equiv I_j/L$ and $z_{\mathcal{S}}(\lambda_\alpha) \equiv J_\alpha/L$. We also defined $\rho(k) \equiv dz_{\mathcal{C}}(k)/dk$ and $\sigma(\lambda) \equiv dz_{\mathcal{S}}(\lambda)/d\lambda$. The symbols $\mathcal{C}(g)$ and $\mathcal{S}(g)$ denote distribution curves on which the quasimomentum k and the rapidity λ lie. By solving Eqs. (3.21) and (3.22) numerically, we obtained the distribution curves $\mathcal{C}(g)$ in the complex k plane for an infinite system as in Fig. 3.3 for $g \le g_{\mathrm{c}}$. We also observed numerically that the distribution curve $\mathcal{S}(g)$ is always located on the real axis from $-\infty$ to ∞ for $g \le g_{\mathrm{c}}$. By differentiating Eqs. (3.21) and (3.22) with respect to k and λ, we have

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_{-\infty}^{\infty} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\sigma(\lambda)d\lambda \qquad \text{for } k \in \mathcal{C}(g), \tag{3.23}$$

$$\sigma(\lambda) = \frac{1}{\pi}\int_{\mathcal{C}(g)} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{U/2t}{(U/2t)^2 + (\lambda-\lambda')^2}\sigma(\lambda')d\lambda' \qquad \text{for } \lambda \in [-\infty, \infty], \tag{3.24}$$

where we assumed $\mathcal{S}(g) = [-\infty, \infty]$. We here consider an area $C_{\mathcal{C}}$ in the k plane as shown in Fig 3.4, where we denote the end points of the curve $\mathcal{C}(g)$ for $g < g_{\mathrm{c}}$ by $\pm\pi + i\kappa(g)$ with $\kappa(g)$ real. The poles of the integrand $(U/4t)/[(U/4t)^2 + (\lambda - \sin k)^2]$ in the k plane get closest to the real axis for $\lambda = 0$:

$$k_n = \pm\,\mathrm{i}\,\mathrm{arcsinh}(U/4t) + n\pi \qquad (n = 0, \pm 1). \tag{3.25}$$

As long as there are no poles in the area $C_{\mathcal{C}}$ shown in Fig. (3.4), we may be able to modify the integral contour $\mathcal{C}(g)$ as [3]

$$\int_{\mathcal{C}(g)} = \int_{-\pi+\mathrm{i}\kappa(g)}^{-\pi} + \int_{-\pi}^{\pi} + \int_{\pi}^{\pi+\mathrm{i}\kappa(g)}, \tag{3.26}$$

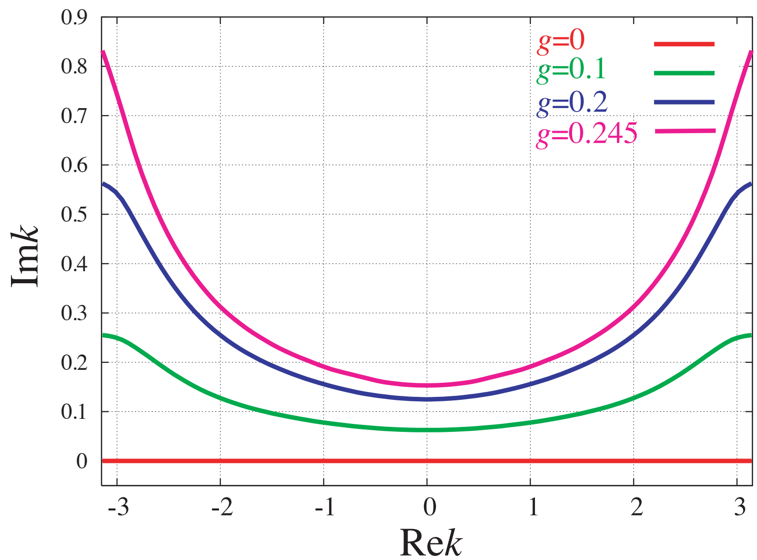


Figure 3.3: The distribution $\mathcal{C}(g)$ of the charge rapidity k for the infinite system with $U/t = 4$. We plot the data for $g = 0, 0.1, 0.2$ and 0.245. The end points become $\pm\pi + i\,0.881\ldots$ as $g \to g_c = 0.246\ldots$.

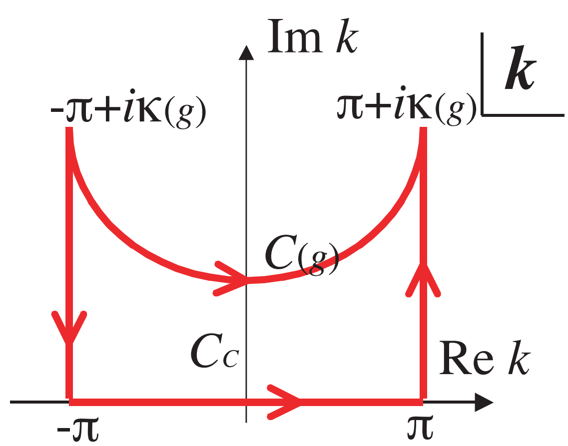


Figure 3.4: The area $C_{\mathcal{C}}$ in the complex k plane.

where we assume that the expression of $\rho(k)$ on the curve $\mathcal{C}(g)$ is valid everywhere inside the area $C_{\mathcal{C}}$ in the complex k plane. The modification of the integral contour $\mathcal{C}(g)$ is thus assumed to be valid as long as the end points $\pm\pi + \mathrm{i}\kappa(g)$ are below the poles at $\pm\pi + \mathrm{i}\,\mathrm{arcsinh}(U/4t)$.

We obtain the non-Hermiticity g at which the end points reach $\pm\pi+\mathrm{i}\,\mathrm{arcsinh}(U/4t)$. The quasimomenta with $\mathrm{Re}\,k = \pm\pi$ may correspond to I_1 and I_N in Eq. (3.19) for $L \to \infty$. Hence we assume $z_{\mathcal{C}}(k) = \pm 1/2$ for the end points of $\mathcal{C}(g)$. We thereby obtain the non-Hermiticity g by substituting $\pm 1/2$ for $z_{\mathcal{C}}(k)$ and $\pm\pi + \mathrm{i}\,\mathrm{arcsinh}(U/4t)$ for k in Eq. (3.21). The result is equal to the non-Hermitian critical point g_{c} in Eq. (3.12), where the charge gap vanishes.

After the above assumption for the modification of the integral counter $\mathcal{C}(g)$, we rewrite Eqs. (3.23) and (3.24) for $g < g_{\mathrm{c}}$ in the forms

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_{-\infty}^{\infty} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\sigma(\lambda)d\lambda \qquad \text{for } k \in [-\pi, \pi], \tag{3.27}$$

$$\begin{aligned}\sigma(\lambda) = {}& \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk + \frac{1}{\pi}\int_{\pi}^{\pi+\mathrm{i}\kappa(g)} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk \\ & + \frac{1}{\pi}\int_{-\pi+\mathrm{i}\kappa(g)}^{-\pi} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{U/2t}{(U/2t)^2 + (\lambda - \lambda')^2}\sigma(\lambda')d\lambda' \\ & \text{for } \lambda \in [-\infty, \infty].\end{aligned} \tag{3.28}$$

Since the integrand is a periodic function with respect to k, we have

$$\frac{1}{\pi}\int_{\pi}^{\pi+\mathrm{i}\kappa(g)} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk + \frac{1}{\pi}\int_{-\pi+\mathrm{i}\kappa(g)}^{-\pi} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk = 0, \tag{3.29}$$

which is followed by

$$\sigma(\lambda) = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho(k)dk - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{U/2t}{(U/2t)^2 + (\lambda - \lambda')^2}\sigma(\lambda')d\lambda' \qquad \text{for } \lambda \in [-\infty, \infty]. \tag{3.30}$$

Equations (3.27) and (3.30) are the same as in the Hermitian case [11]. The solutions are obtained by taking the Fourier transformation of $\sigma(\lambda)$ and are given by [11]

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_0^{\infty} \frac{\cos(\omega \sin k)J_0(\omega)}{1 + e^{\omega U/2t}}d\omega \qquad \text{for } k \in [-\pi, \pi], \tag{3.31}$$

$$\sigma(\lambda) = \frac{1}{2\pi}\int_0^{\infty} \mathrm{sech}\left(\frac{U}{4t}\omega\right)\cos(\lambda\omega)J_0(\omega)d\omega \qquad \text{for } \lambda \in [-\infty, \infty]. \tag{3.32}$$

The above suggests that the analytic continuation of the solutions $\rho(k)$ and $\sigma(\lambda)$ may be valid inside the area $C_{\mathcal{C}}(g_{\mathrm{c}})$, where $C_{\mathcal{C}}(g_{\mathrm{c}})$ is the area $C_{\mathcal{C}}$ for $g = g_{\mathrm{c}}$.

Eigenenergies

We calculate the dependence of eigenenergies on the non-Hermiticity g in the region $g < g_{\mathrm{c}}$, particularly, the ground-state energy and the charge excitation energy.

We first obtain the ground state energy E_{gs}. As long as there are no poles in $C_{\mathcal{C}}$ in Fig. 3.4, that is, for $g < g_{\mathrm{c}}$, the ground state energy E_{gs} per site is

$$\begin{aligned} E_{\mathrm{gs}}(g) &= -2t \int_{\mathcal{C}(g)} \cos k \rho(k) dk \\ &= -2t \int_{-\pi}^{\pi} \cos k \rho(k) dk - 2t \int_{-\pi}^{-\pi+\mathrm{i}\kappa(g)} \cos k \rho(k) dk - 2t \int_{\pi}^{\pi+\mathrm{i}\kappa(g)} \cos k \rho(k) dk. \end{aligned} \tag{3.33}$$

Since $\cos k \rho(k)$ is a periodic function with respect to k, we have

$$-2t \int_{-\pi}^{-\pi+\mathrm{i}\kappa(g)} \cos k \rho(k) dk - 2t \int_{\pi}^{\pi+\mathrm{i}\kappa(g)} \cos k \rho(k) dk = 0. \tag{3.34}$$

Hence $E_{\mathrm{gs}}(g)$ is given by

$$E_{\mathrm{gs}}(g) = -2t \int_{-\pi}^{\pi} \cos k \rho(k) dk = -4t \int_0^{\infty} \frac{J_0(\omega) J_1(\omega)}{\omega(1+e^{\omega U/2t})} d\omega. \tag{3.35}$$

We thus find that the ground state energy does not depend on g for $g < g_{\mathrm{c}}$.

We next obtain the excitation energy $\mathcal{E}(k_h)$ on the curve $\mathcal{C}(g)$. The excitation energy is defined in terms of the chemical potentials μ_+ and μ_- in the form [11]

$$\mathcal{E}(k_h) \equiv \mu_+ - \mu_-, \tag{3.36}$$

where μ_+ is the chemical potential as we take one electron in and μ_- is the one as we take one electron out at the quasimomentum k_h. Specifically, μ_+ and μ_- are defined as

$$\begin{aligned} \mu_+ &\equiv E(M+1, M) - E(M, M), \\ \mu_- &\equiv E(M, M) - E(M-1, M), \end{aligned} \tag{3.37}$$

where $E(n_\uparrow, n_\downarrow)$ denotes the eigenenergy in the subspace where the numbers of the up spins and the down spins are $n_\uparrow$ and $n_\downarrow$, respectively. By considering the particle-hole transformation:

$$\begin{aligned} c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger |\mathrm{vac}\rangle \quad &\to \quad |\mathrm{vac}\rangle, \\ |\mathrm{vac}\rangle \quad &\to \quad c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger |\mathrm{vac}\rangle, \end{aligned} \tag{3.38}$$

we have

$$E(L-n_\uparrow, L-n_\downarrow) - E(n_\uparrow, n_\downarrow) = (n_{\mathrm{double}} - n_{\mathrm{vac}})U = (L - n_\uparrow - n_\downarrow)U, \tag{3.39}$$

where n_{double} and n_{vac} are the number of double occupancies and the number of the vacuum states, respectively. By using Eq. (3.39), we rewrite μ_+ in the form

$$\begin{aligned} \mu_+ =& E(M+1, M) - E(M, M) \\ =& E(L-(M+1), L-M) - [L-(M+1)-M]U - E(M, M) \\ =& E(M-1, M) - E(M, M) + U = -\mu_- + U. \end{aligned} \tag{3.40}$$

Hence we have the excitation energy $\mathcal{E}(k_h)$ at the quasimomentum k_h of the form

$$\mathcal{E}(k_h) = U - 2\mu_-. \tag{3.41}$$

For the calculation of μ_-, we remove an electron whose quasimomentum is k_h. The distribution of I_j changes into

$$I_j = \frac{N-1}{2}, \ldots, \frac{N-2h+3}{2}, \frac{N-2h-1}{2}, \ldots, -\frac{N-1}{2}, \tag{3.42}$$

where we remove the $(h-1)$th quantum number. We assume that the distribution function $\rho(k)$ in Eqs. (3.23) and (3.24) for the ground state changes into $\rho_h(k) - \frac{1}{L}\delta(k-k_h)$ by the one-hole excitation at $k = k_h$ on the distribution curve $\mathcal{C}(g)$. The Bethe-ansatz equation then becomes

$$\begin{aligned}
\rho_h(k) &= \frac{1}{2\pi} - \frac{1}{L}\delta(k-k_h) + \frac{\cos k}{\pi}\int_{\mathcal{S}(g)} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\sigma_h(\lambda)d\lambda \qquad \text{for } k \in \mathcal{C}(g),\\
\sigma_h(\lambda) &= \frac{1}{\pi}\int_{\mathcal{C}(g)} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho_h(k)dk - \frac{1}{\pi}\int_{\mathcal{S}(g)} \frac{U/2t}{(U/2t)^2 + (\lambda - \lambda')^2}\sigma_h(\lambda')d\lambda'\\
&\qquad \text{for } \lambda \in \mathcal{S}(g).
\end{aligned} \tag{3.43}$$

As long as g is less than the non-Hermitian critical point g_c, we assume to be able to modify the integral counters $\int_{\mathcal{C}(g)}$ as Eq. (3.26) and $\int_{\mathcal{S}}$ as $\int_{-\infty}^{\infty}$, where we assume that the expression of $\rho_h(k)$ on the curve $\mathcal{C}(g)$ is valid everywhere inside the area $C_{\mathcal{C}}$ in the complex k plane. Since the integrands in Eq. (3.43) have the periodicity 2π with respect to k, we can reduce the integral counter in Eq. (3.26) to $\int_{-\pi}^{\pi}$. The modified Bethe-ansatz equation then becomes

$$\begin{aligned}
\rho_h(k) &= \frac{1}{2\pi} - \frac{1}{L}\delta(k-k_h) + \frac{\cos k}{\pi}\int_{-\infty}^{\infty} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\sigma_h(\lambda)d\lambda \qquad \text{for } k \in [-\pi,\pi],\\
\sigma_h(\lambda) &= \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{U/4t}{(U/4t)^2 + (\lambda - \sin k)^2}\rho_h(k)dk - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{U/2t}{(U/2t)^2 + (\lambda - \lambda')^2}\sigma_h(\lambda')d\lambda'\\
&\qquad \text{for } \lambda \in [-\infty,\infty].
\end{aligned} \tag{3.44}$$

The solutions of Eq. (3.44) are obtained by taking the Fourier transformation of $\sigma(\lambda)$ and are given by

$$\begin{aligned}
\sigma_h(\lambda) =& \frac{1}{\pi}\int_0^{\infty} \operatorname{sech}\left(\frac{U}{4t}\omega\right)\cos(\lambda\omega)J_0(\omega)d\omega - \frac{t}{UL}\operatorname{sech}\left[\frac{2\pi t}{U}(\lambda - \sin k_h)\right]\\
&\qquad \text{for } \lambda \in [-\infty,\infty],\\
\rho_h(k) =& \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_0^{\infty} \frac{\cos(\omega \sin k)J_0(\omega)}{1 + e^{\omega U/2t}} - \frac{1}{L}\delta(k-k_h)\\
&- \frac{\cos k}{\pi L}\int_0^{\infty} \frac{\cos[\omega(\sin k - \sin k_h)]}{1+e^{\omega U/2t}}d\omega \qquad \text{for } k \in [-\pi,\pi],
\end{aligned} \tag{3.45}$$

where we here assume that the analytic continuation of $\rho_h(k)$ is valid everywhere inside the area $C_{\mathcal{C}}$. Since the integral of the distribution function of the charge excitation changes by $1/L$, we pick out the excitation as the shift of $\rho_h(k)$ in the order of $1/L$. This has the form

$$\Delta\rho_h(k) \equiv -\delta(k-k_h) - \frac{\cos k}{\pi}\int_0^\infty \frac{\cos[\omega(\sin k - \sin k_h)]}{1+e^{\omega U/2t}}d\omega \tag{3.46}$$

everywhere inside the area $C_{\mathcal{C}}$. We thus obtain the chemical potential μ_-;

$$\begin{aligned}\mu_- &\equiv -2t\int_{\mathcal{C}(g)} \cos k\Delta\rho_h(k)dk = -2t\int_{-\pi}^{\pi} \cos k\Delta\rho_h(k)dk \\ &= -2\cos k_h - 4t\int_0^\infty \frac{\cos(\omega\sin k_h)J_1(\omega)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega.\end{aligned} \tag{3.47}$$

We therefore obtain the excitation energy $\mathcal{E}(k_h)$ on the curve $\mathcal{C}(g)$:

$$\mathcal{E}(k_h) = U + 4t\cos k_h + 8t\int_0^\infty \frac{\cos(\omega\sin k_h)J_1(\omega)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega. \tag{3.48}$$

We note that the excitation energy in Eq. (3.48) has the same expression as in the Hermitian case (3.7). In short, the analytic continuation of the expression $\mathcal{E}(k_h)$ in Eq. (3.7) is considered to be valid in the area $C_{\mathcal{C}}(g_c)$ in the complex k plane as we assume that the expression of $\rho_h(k)$ is valid everywhere inside the area $C_{\mathcal{C}}$. (Note, however, that k_h is on $\mathcal{C}(g)$ and hence depends on g.)

We next discuss how the Hubbard gap vanishes as we increase the non-Hermiticity g. In the non-Hermitian case, we define the "Hubbard gap" as the excitation energy at the end point $k_h = \pm\pi + \mathrm{i}\kappa$ on the curve $\mathcal{C}(g)$. The dependence of the Hubbard gap $\Delta_{\mathrm{Hubbard}}$ on κ is

$$\begin{aligned}\Delta_{\mathrm{Hubbard}} &= \mathcal{E}(k_h = \pm\pi + \mathrm{i}\kappa) \\ &= U - 4t\cosh\kappa + 8t\int_0^\infty \frac{\cosh(\omega\sinh\kappa)J_1(\omega)}{\omega(1+e^{\omega U/2t})}d\omega.\end{aligned} \tag{3.49}$$

From Eq. (3.21), on the other hand, the dependence of the non-Hermiticity g on κ is

$$g(\kappa) = \kappa - 2\int_0^\infty \frac{\sinh(\omega\sinh\kappa)J_0(\omega)}{\omega(1+e^{\omega U/2t})}d\omega. \tag{3.50}$$

We thus obtain the dependence of the Hubbard gap on the non-Hermiticity g through the parameter κ. Figure 3.5 numerically exemplifies how the Hubbard gap collapses as we increase the non-Hermiticity g. The ground-state energy does not change and the Hubbard gap gradually decreases before it vanishes at $g = g_c$. The way the energy gap collapses is different from that for the Anderson model discussed by Hatano and Nelson [2]; the difference of the order of $1/L$ between neighboring eigenvalues decreases almost suddenly as g gets close to $g = g_c$ [5].

We here comment that the Hubbard gap $\Delta_{\mathrm{Hubbard}}$ has a singularity with an exponent $1/2$

$$\Delta_{\mathrm{Hubbard}} \sim c(g_c - g)^{1/2} + \mathrm{O}(g_c - g) \tag{3.51}$$

around but below the non-Hermitian critical point $g = g_c$, where c is a positive constant given below. We consider the Taylor expansion of the Hubbard

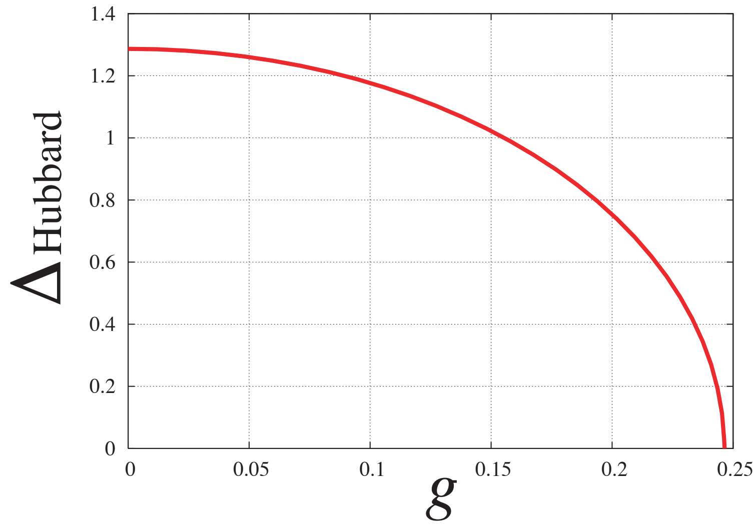


Figure 3.5: The g dependence of the Hubbard gap Δ_{Hubbard} for $U/t = 4$. The non-Hermitian critical point is $g_{\text{c}} \cong 0.246$.

gap Δ_{Hubbard} in Eq. (3.49) and the non-Hermiticity $g(\kappa)$ in Eq. (3.50) around $\kappa = \kappa(g_{\text{c}})(\equiv \text{arcsinh}(U/4t))$ which determines the non-Hermitian critical point g_{c}:

$$\Delta_{\text{Hubbard}} = 4t\sqrt{(U/4t)^2+1}\left(1-2\sum_{n=1}^{\infty}(-1)^n\frac{(2n-1)(U/4t)}{\sqrt{(2n-1)^2(U/4t)^2+1}}\right)(\kappa_{\text{c}}-\kappa)+\text{O}\left((\kappa_{\text{c}}-\kappa)^2\right),$$
$$g(\kappa) = g_{\text{c}} + 2\left[(U/4t)^2+1\right]\sum_{n=1}^{\infty}(-1)^n\frac{(2n-1)(U/4t)}{\left[(2n-1)^2(U/4t)^2+1\right]^{3/2}}(\kappa_{\text{c}}-\kappa)^2+\text{O}\left((\kappa_{\text{c}}-\kappa)^3\right). \tag{3.52}$$

These expressions are assumed to be valid for $\kappa \leq \kappa(g_{\text{c}})$. We thus obtain the asymptotic behavior around $g \sim g_{\text{c}}$ in the form Eq. (3.51) with

$$c = 2\sqrt{2}t\frac{1-2\displaystyle\sum_{n=1}^{\infty}(-1)^n\frac{(2n-1)(U/4t)}{\sqrt{(2n-1)^2(U/4t)^2+1}}}{\sqrt{\displaystyle\sum_{n=1}^{\infty}(-1)^{n+1}\frac{(2n-1)(U/4t)}{[(2n-1)^2(U/4t)^2+1]^{3/2}}}}. \tag{3.53}$$

We later argue that the non-Hermitian $S = 1/2$ antiferromagnetic XXZ chain (4.15) has the same exponent 1/2.

For $g \geq g_{\text{c}}$, on the other hand, Fukui and Kawakami [3] argued the shapes of the distribution curves $\mathcal{C}$ and $\mathcal{S}$ are quite different from the ones in the region $g < g_{\text{c}}$. Bethe-ansatz equations thus do not become the Hermitian ones at all. It is therefore difficult to know ground-state properties of the non-Hermitian Hubbard model (3.11) for $g \geq g_{\text{c}}$. However, we expect that the ground-state energy becomes complex for $g > g_{\text{c}}$ on the basis of finite-size data shown in §6.1.

3.2.2 Physical meaning of the non-Hermitian generalization

We argue physical meaning of the non-Hermitian generalization of the Hubbard model; the non-Hermiticity g makes the dispersion relation $\mathcal{E}(p_h)$ of the charge excitation at the momentum p_h transformed to $\mathcal{E}(p_h + ig)$.

For the non-Hermitian Hubbard model (3.11), let us first obtain the momentum $p_h(g)$ of the hole at the quasimomentum k_h, or, at the quantum number I_h in Eq. (3.42) defined [9] as

$$p_h(g) \equiv \sum_{j=1}^{N} k_j^{\mathrm{gs}} - \sum_{j=1}^{N-1} k_j^{\mathrm{es}} = \frac{2\pi I_h}{L} = 2\pi z_{\mathcal{C}}(k_h), \tag{3.54}$$

where $\{k_j^{\mathrm{gs}}\}$ denotes the set of the quasimomenta for the ground state and $\{k_j^{\mathrm{es}}\}$ denotes the one for the excited state due to the charge excitation at $k_j^{\mathrm{gs}} = k_h$. From Eq. (3.21), we have

$$\begin{aligned} g &= 2\pi \mathrm{i} z_{\mathcal{C}}(k_h) - \mathrm{i}k_h - \mathrm{i}\int_{-\infty}^{\infty} 2\arctan\frac{\sin k_h - \lambda}{U/4t}\sigma(\lambda)d\lambda \\ &= 2\pi \mathrm{i} z_{\mathcal{C}}(k_h) - \mathrm{i}k_h - 2\mathrm{i}\int_{0}^{\infty} \frac{\sin(\omega \sin k_h)J_0(\omega)}{\omega(1+e^{\omega U/2t})}d\omega \\ &\equiv 2\pi \mathrm{i} z_{\mathcal{C}}(k_h) - \mathrm{i}P_h, \end{aligned} \tag{3.55}$$

where P_h denotes the momentum $p(k_h)$ of the hole given by Eq. (3.8). Since the analytic continuation of the excitation energy $\mathcal{E}(k_h)$ or $\mathcal{E}(p(k_h)) = \mathcal{E}(P_h)$ is assumed to be valid for $g < g_{\mathrm{c}}$ as shown in Eq. (3.48), the non-Hermitian Hamiltonian (3.11) may be diagonalized in low energy in the form

$$\mathcal{H}_{\mathrm{Hubbard}}(g) \cong \sum_{-\pi < p_h(g) < \pi} \mathcal{E}(P_h)\eta^{\dagger}_{p_h(g)}\eta_{p_h(g)} \tag{3.56}$$

in terms of the charge excitation, where $\eta^{\dagger}_{p_h(g)}$ and $\eta_{p_h(g)}$ are the creation and annihilation operators of the hole at the momentum $p_h(g)$. The Hamiltonian (3.56) is rewritten in the form

$$\mathcal{H}_{\mathrm{Hubbard}}(g) \cong \sum_{-\pi < p_h(g) < \pi} \mathcal{E}(p_h(g) + ig)\eta^{\dagger}_{p_h(g)}\eta_{p_h(g)} \tag{3.57}$$

because we have $P_h = p_h(g) + ig$ from Eq. (3.55). Since $p_h(g)$ is real, Eq. (3.57) has the same structure as Eqs. (1.6) and (2.15). We thus conclude that we may be able to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$ in the complex momentum p space by analyzing the non-Hermitian Hamiltonian (3.11).

The assumption that the analytic continuation of the excitation energy is valid everywhere inside the area $C_{\mathcal{C}}$ in the complex quasimomentum space is equivalent to the assumption that the analytic continuation of the dispersion relation is valid in the area

$$\mathrm{Im}\, p < g_{\mathrm{c}} \tag{3.58}$$

in the complex momentum space. The zeros of the dispersion relation of the charge excitation for the Hermitian Hubbard model in Eq. (3.10) indeed exist in the region (3.58).

Chapter 4

$S = 1/2$ antiferromagnetic $\boldsymbol{XXZ}$ chain

In the present chapter, we consider the $S = 1/2$ antiferromagnetic XXZ chain

$$\mathcal{H}_{XXZ} = J \sum_{l=1}^{L} \left[\frac{1}{2} \left(S_l^- S_{l+1}^+ + S_l^+ S_{l+1}^- \right) + \Delta S_l^z S_{l+1}^z \right] \tag{4.1}$$

in the Ising-like region $\Delta > 1$ for $J > 0$, whose ground state has an energy gap above it due to the spinon excitation.

4.1 Zeros of the dispersion relation of the spinon excitation and the correlation length

We first point out that the imaginary part of zeros in the complex momentum space of the dispersion relation of the two-spinon excitation is equal to twice the inverse correlation length of the spinon excitation. A pair of spinon excitations at the rapidities $\lambda = \lambda_1$ and $\lambda = \lambda_2$ has the excitation energy of the form

$$\begin{aligned} \mathcal{E}(\lambda_1, \lambda_2) &= \frac{2\pi J \sinh\gamma}{\gamma} \left(\sigma(\lambda_1) + \sigma(\lambda_2) \right) \\ &= \frac{J \sinh\gamma K(u)}{\pi} \left[\mathrm{dn}\left(\frac{\gamma K(u) \lambda_1}{\pi}, u \right) + \mathrm{dn}\left(\frac{\gamma K(u) \lambda_2}{\pi}, u \right) \right], \end{aligned} \tag{4.2}$$

where the distribution function $\sigma(\lambda)$ of the rapidity λ is given by

$$\sigma(\lambda) = \frac{\gamma}{2\pi} \sum_{n=-\infty}^{n=\infty} \frac{e^{in\gamma\lambda}}{2\cosh(n\gamma)} = \frac{\gamma K(u)}{2\pi^2} \mathrm{dn}\left(\frac{\gamma K(u) \lambda}{\pi}, u \right) \tag{4.3}$$

and we set $\gamma = \mathrm{arccosh}\Delta$. The functions $\mathrm{dn}(x, u)$ in Eqs. (4.2) and (4.3) and $\mathrm{sn}(x, u)$ in Eq. (4.8) are the Jacobian elliptic functions. The modulus u is determined by

$$\frac{K(\sqrt{1-u^2})}{K(u)} = \frac{\gamma}{\pi}, \tag{4.4}$$

where $K(u)$ is defined by

$$K(u) \equiv \int_0^{\pi/2} \frac{dp}{\sqrt{1-u^2\sin^2 p}}. \tag{4.5}$$

By considering Eqs. (4.4) and (4.5), the modulus u is given by

$$u = \left[\cosh\left(\frac{\gamma}{2} + \sum_{n=1}^{\infty} \frac{(-1)^n \tanh(n\gamma)}{n}\right)\right]^{-1}. \tag{4.6}$$

The momentum $p_{\rm spinon}$ of the two-spinon excitation is

$$p_{\rm spinon} = p(\lambda_1) + p(\lambda_2), \tag{4.7}$$

where

$$p(\lambda) \equiv \frac{\gamma\lambda}{2} + \sum_{n=1}^{\infty} \frac{\sin(n\gamma\lambda)}{n\cosh(n\gamma)} = \arcsin\left[\mathrm{sn}\left(\frac{\gamma K(u)\lambda}{\pi}, u\right)\right]. \tag{4.8}$$

By using the formula $\mathrm{dn}(x,u) = \sqrt{1-u^2\mathrm{sn}^2(x,u)}$, we obtain the explicit expression of the dispersion relation $\mathcal{E}(\lambda_1,\lambda_2)$ as a function of $p(\lambda_1)$ and $p(\lambda_2)$ of the form

$$\mathcal{E}(\lambda_1,\lambda_2) = \frac{J\sinh\gamma K(u)}{\pi}\left[\sqrt{1-u^2\sin^2 p(\lambda_1)} + \sqrt{1-u^2\sin^2 p(\lambda_2)}\right]. \tag{4.9}$$

We search zeros of $\mathcal{E}(\lambda_1,\lambda_2)$ by considering the analytic continuation of the dispersion relation of the spinon excitation. Because of Eq. (4.9), the zeros $p^{(0)}(\lambda_1)$ and $p^{(0)}(\lambda_2)$ with $\mathcal{E}(\lambda_1^{(0)},\lambda_2^{(0)}) = 0$ must satisfy

$$\sin p^{(0)}(\lambda_i) = \pm\frac{1}{u} \tag{4.10}$$

for $i = 1$ and 2. All zeros $p^{(0)}(\lambda_1)$ and $p^{(0)}(\lambda_2)$ in the regions $\mathrm{Im}\, p(\lambda_1) \geq 0$ and $\mathrm{Im}\, p(\lambda_2) \geq 0$ are thus given by

$$p^{(0)}(\lambda_1),\ p^{(0)}(\lambda_2) = \pm\frac{\pi}{2} + \mathrm{i}\,\mathrm{arccosh}\left(\frac{1}{u}\right) = \pm\frac{\pi}{2} + \mathrm{i}\left[\frac{\gamma}{2} + \sum_{n=1}^{\infty}\frac{(-1)^n\tanh(n\gamma)}{n}\right]. \tag{4.11}$$

All zeros $p_{\rm spinon}^{(0)}$ of the momentum of the two spinon excitation in the region $\mathrm{Im}\, p_{\rm spinon} \geq 0$ are

$$p_{\rm spinon}^{(0)} = \pm\,\pi + \mathrm{i}\left[\gamma + 2\sum_{n=1}^{\infty}\frac{(-1)^n\tanh(n\gamma)}{n}\right], \quad \mathrm{i}\left[\gamma + 2\sum_{n=1}^{\infty}\frac{(-1)^n\tanh(n\gamma)}{n}\right]. \tag{4.12}$$

We note that the imaginary part of the momentum in Eq. (4.12) is equal to *twice* the inverse correlation length $1/\xi$ obtained by the quantum transfer matrix method of the form [14]

$$\frac{1}{\xi} = \frac{\gamma}{2} + \sum_{n=1}^{\infty}\frac{(-1)^n\tanh(n\gamma)}{n}, \tag{4.13}$$

that is,

$$p^{(0)}_{\text{spinon}} = \pm\pi + 2\mathrm{i}/\xi, \quad 2\mathrm{i}/\xi. \tag{4.14}$$

The reason why $\operatorname{Im} p^{(0)}_{\text{spinon}}$ is equal to *twice* the inverse correlation length in Eq. (4.14) is that we consider a two-spinon excitation. The above relation was first pointed out by Okunishi *et al.* [15] for the $S = 1/2$ XYZ chain. However, they did not discuss where in the complex momentum space the analytic continuation is valid. We argue below by analyzing the non-Hermitian $S = 1/2$ XXZ chain that the zeros $\pm\pi + 2\mathrm{i}/\xi$ and $2\mathrm{i}/\xi$ in the complex momentum space actually exist in the area where the analytic continuation is assumed to be valid.

4.2 Non-Hermitian analysis of the antiferromagnetic *XXZ* chain

For the purpose of searching zeros in the complex momentum space, we use a non-Hermitian XXZ chain in order to obtaining the dispersion relation on the axis $\operatorname{Im} p = g$ with real g. As will be demonstrated in §4.2.2, obtaining the dispersion relation on the axis $\operatorname{Im} p = g$ may be equivalent to solving a non-Hermitian XXZ chain [16]

$$\mathcal{H}_{XXZ}(g) = J \sum_{l=1}^{L} \left[\frac{1}{2} \left(e^{2g} S_l^- S_{l+1}^+ + e^{-2g} S_l^+ S_{l+1}^- \right) + \Delta S_l^z S_{l+1}^z \right] \tag{4.15}$$

with $J > 0$. We set $S^z_{\text{tot}} = 0$ hereafter. The non-Hermitian Hamiltonian $\mathcal{H}_{XXZ}(g)$ in the case of $\Delta = 1$ is derived as an effective Hamiltonian in the strong coupling expansion of the non-Hermitian Hubbard model in the half-filled case,

$$\mathcal{H}_{\text{spin}}(g) = -t \sum_{l=1}^{L} (e^g c^\dagger_{l+1,\uparrow} c_{l,\uparrow} + e^{-g} c^\dagger_{l,\uparrow} c_{l+1,\uparrow} + e^{-g} c^\dagger_{l+1,\downarrow} c_{l,\downarrow} + e^g c^\dagger_{l,\downarrow} c_{l+1,\downarrow}) + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}, \tag{4.16}$$

which is a special case $t' = 0$ of the model (E.1) in Appendix E. Note the difference between Eqs. (3.11) and (4.16); the first-order perturbation with respect to the non-Hermiticity g gives

$$\mathcal{H}_{\text{spin}}(g) - \mathcal{H}_{\text{spin}}(0) = -\mathrm{i}g(J_\uparrow - J_\downarrow), \tag{4.17}$$

where $J_\uparrow - J_\downarrow$ is the spin current operator. Thus we expect that the non-Hermiticity g induces a spin current and eliminates the spin gap. We then generalize the model to arbitrary values of Δ.

Albertini *et al.* [16] exactly solved the non-Hermitian XXZ chain (4.15) and obtained an analytical expression in the limit $L \to \infty$ of the non-Hermitian critical point g_{c} at which the energy gap due to the spinon excitation vanishes, in the form [16]

$$g_{\text{c}} = \frac{\gamma}{2} + \sum_{n=1}^{\infty} \frac{(-1)^n \tanh(n\gamma)}{n}. \tag{4.18}$$

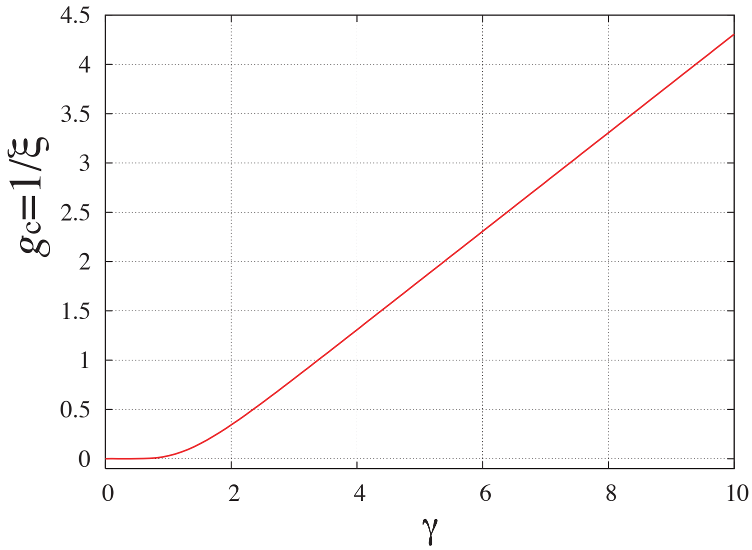


Figure 4.1: The γ dependence of $g_c = \xi^{-1}$.

We show the γ dependence of g_c in Fig. 4.1. Although Albertini *et al.* did not point out the fact, the expression (4.18) is the same as Eq. (4.13). We demonstrate below that zeros $p^{(0)}_{\text{spinon}}$ in Eq. (4.14) actually exist in the area where the analytic continuation is assumed to be valid by analyzing the non-Hermitian *XXZ* chain (4.15). In §4.2.1, we review the analytic solution [16] of the non-Hermitian Hamiltonian (4.15) by the Bethe-ansatz method. In §4.2.2, we argue physical meaning of the non-Hermitian generalization of the *XXZ* chain; the non-Hermiticity g makes the dispersion relation $\mathcal{E}(p)$ of a spinon transformed to $\mathcal{E}(p + ig)$.

4.2.1 Exact solution of the antiferromagnetic non-Hermitian *XXZ* chain

Bethe-ansatz equation and its exact solution

We now consider the case of zero magnetization $\sum_{i=1}^{L} S_i^z = 0$ with even L, M up spins and M down spins ($M \equiv L/2$). We define the vacuum state $|\text{vac}\rangle$ as the state where all spins are up. An eigenfunction with M down spins is given by

$$|\Psi^{(\text{R})}(g)\rangle = \sum_{(x_1, x_2, \cdots, x_M)} \psi_g^{(\text{R})}(x_1, x_2, \cdots, x_M) S^-_{x_1} S^-_{x_2} \cdots S^-_{x_M} |\text{vac}\rangle, \tag{4.19}$$

where we put down spins at $x_1, x_2, \cdots, x_M$ with $1 \le x_1 \le x_2 \le \cdots \le x_M \le L$. In order to solve the non-Hermitian Hamiltonian (4.15), we make the following ansatz for the right eigenfunction $\psi_g^{(\mathrm{R})}$ [16]:

$$\begin{aligned}\psi_g^{(\mathrm{R})}(x_1, x_2, \cdots, x_M) &= \exp\left(2g\sum_{j=1}^{M} x_j\right)\psi_0(x_1, x_2, \cdots, x_M) \\ &= \sum_{\{P\}} A(P_1, \cdots, P_M)\exp(\mathrm{i}\sum_{j=1}^{M}(k_{P_j} - 2\mathrm{i}g)x_j).\end{aligned} \tag{4.20}$$

The wave function ψ_0 is the Bethe-ansatz wave function in the Hermitian case $g = 0$:

$$\psi_0(x_1, x_2, \cdots, x_M) = \sum_{\{P\}} A(P_1, \cdots, P_M)\exp(\mathrm{i}\sum_{j=1}^{M} k_{P_j} x_j), \tag{4.21}$$

where the symbol $P = (P_1, P_2, \cdots, P_M)$ denotes a permutation of the set $(1, 2, \cdots, M)$. The symbol $A(P_1, \cdots, P_M)$ is a set of $M!$ coefficients depending on the permutation P. The quasimomenta $k_1, k_2, \cdots, k_M$ are unequal to each other for the ground state.

The Schrödinger equation for $\psi_g^{(\mathrm{R})}$ is

$$\begin{aligned}&\frac{J}{2}\sum_{j=1}^{M}(1 - \delta_{x_j+1, x_{j+1}})\left[e^{-2g}\psi_g^{(\mathrm{R})}(x_1, \cdots, x_j + 1, \cdots, x_M) + e^{2g}\psi_g^{(\mathrm{R})}(x_1, \cdots, x_{j+1} - 1, \cdots, x_M)\right] \\ &+ \left[\Delta J\sum_{j=1}^{M}\delta_{x_j+1, x_{j+1}} + \Delta J\left(\frac{L}{4} - M\right)\right]\psi_g^{(\mathrm{R})}(x_1, \cdots, x_M) = E\psi_g^{(\mathrm{R})}(x_1, \cdots, x_M),\end{aligned} \tag{4.22}$$

where E is an eigenenergy. The Schrödinger equation (4.22) yields

$$E = J\sum_{j=1}^{M}(\cos k_j - \Delta) + \frac{\Delta J}{4}L, \tag{4.23}$$

$$\frac{A(P_1, \cdots, P_{j+1}, P_j, \cdots, P_M)}{A(P_1, \cdots, P_j, P_{j+1}, \cdots, P_M)} = (-1)\frac{1 + \exp[\mathrm{i}(k_{P_j} + k_{P_{j+1}})] - 2\Delta\exp(\mathrm{i}k_{P_{j+1}})}{1 + \exp[\mathrm{i}(k_{P_j} + k_{P_{j+1}})] - 2\Delta\exp(\mathrm{i}k_{P_j})}. \tag{4.24}$$

The periodic boundary condition $\psi_g^{(\mathrm{R})}(x_1, x_2, \cdots, x_M) = \psi_g^{(\mathrm{R})}(x_2, \cdots, x_M, x_1 + L)$ yields the Bethe-ansatz equation for $1 \leq j \leq M$ [16]:

$$\exp(\mathrm{i}k_j L + 2gL) = (-1)^{M-1}\prod_{l\neq j}^{M}\frac{\exp[\mathrm{i}(k_j + k_l)] + 1 - 2\Delta\exp(\mathrm{i}k_j)}{\exp[\mathrm{i}(k_j + k_l)] + 1 - 2\Delta\exp(\mathrm{i}k_l)}. \tag{4.25}$$

We here introduce a new rapidity parameter λ_j:

$$\exp(\mathrm{i}k_j) = -\frac{\sin[\gamma(\lambda_j + \mathrm{i})/2]}{\sin[\gamma(\lambda_j - \mathrm{i})/2]}. \tag{4.26}$$

Equation (4.25) then becomes

$$\left[\frac{\sin\frac{\gamma}{2}(\lambda_j + \mathrm{i})}{\sin\frac{\gamma}{2}(\lambda_j - \mathrm{i})}\right]^L e^{2gL} = \prod_{l\neq j}^{M}\frac{\sin\frac{\gamma}{2}(\lambda_j - \lambda_l + 2\mathrm{i})}{\sin\frac{\gamma}{2}(\lambda_j - \lambda_l - 2\mathrm{i})}. \tag{4.27}$$

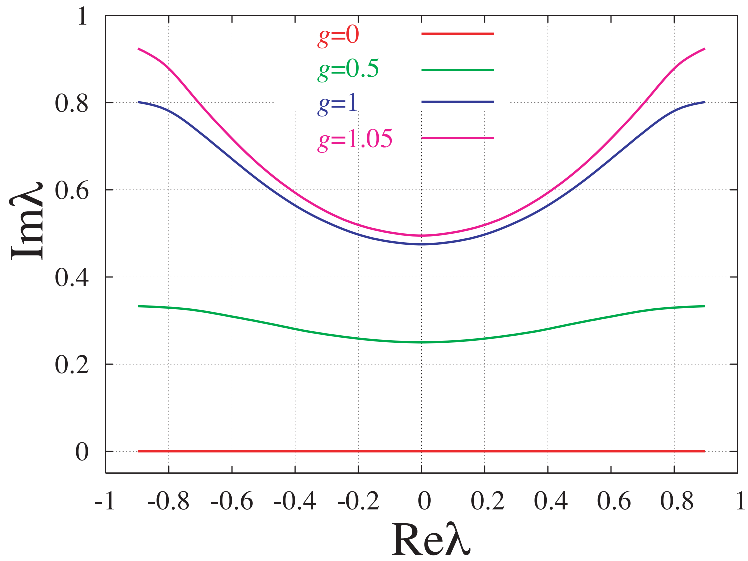


Figure 4.2: The distribution curve of the spin rapidity λ for the infinite system with $\gamma = 3.5$. In this case, the non-Hermitian critical point $g_c \simeq 1.05867$.

By taking the logarithm of Eq. (4.27), we have

$$2L \arctan\left[\frac{\tan(\gamma\lambda_j/2)}{\tanh(\gamma/2)}\right] = 2\pi I_j + 2igL + 2\sum_{l=1}^{M} \arctan\left[\frac{\tan[\gamma(\lambda_j - \lambda_l)/2]}{\tanh(\gamma)}\right], \quad (4.28)$$

where the quantum number I_j for the ground state for $L = 4n - 2$ ($n \in \mathbf{N}$) is given by

$$I_j = \frac{L/2-1}{2}, \frac{L/2-3}{2}, \cdots, -\frac{L/2-1}{2}. \quad (4.29)$$

The summation in Eq. (4.28) becomes an integral in the limit $L \to \infty$ as

$$\underbrace{2\arctan\left[\frac{\tan(\gamma\lambda/2)}{\tanh(\gamma/2)}\right]}_{\equiv\theta_1(\lambda)} = 2\pi z_s(\lambda) + 2ig + 2\int_{\mathcal{S}(g)} \underbrace{\arctan\left[\frac{\tan[\gamma(\lambda-\Lambda)/2]}{\tanh(\gamma)}\right]}_{\equiv\theta_2(\lambda-\Lambda)} \sigma(\Lambda) d\Lambda \quad (4.30)$$

for $\lambda \in \mathcal{S}(g)$, where $\mathcal{S}(g)$ denotes the distribution curve in the complex λ plane on which the rapidity λ lies; see Fig. 4.2 for numerical calculation. In Eq. (4.30), we introduced a function $z_{\mathcal{S}}(\lambda)$ by taking the continuous limit $L \to \infty$ of the discrete function $z_{\mathcal{S}}(\lambda_\alpha) \equiv J_\alpha/L$. We also define $\sigma(\lambda) \equiv dz_{\mathcal{S}}(\lambda)/d\lambda$. We restrict ourselves to the region $-\pi/\gamma \le \mathrm{Re}\,\lambda \le \pi/\gamma$, since $\theta_1(\lambda)$ in Eq. (4.30) is a function of the periodicity $2\pi/\gamma$.

The distribution function $\sigma(\lambda)$ satisfies the following integral equation after differentiating Eq. (4.30) with respect to λ:

$$\frac{\gamma\sinh\gamma}{\cosh\gamma - \cos\gamma\lambda} = 2\pi\sigma(\lambda) + \int_{\mathcal{S}(g)} \frac{\gamma\sinh(2\gamma)}{\cosh(2\gamma) - \cos\{\gamma(\lambda-\Lambda)\}}\sigma(\Lambda)d\Lambda \quad (4.31)$$

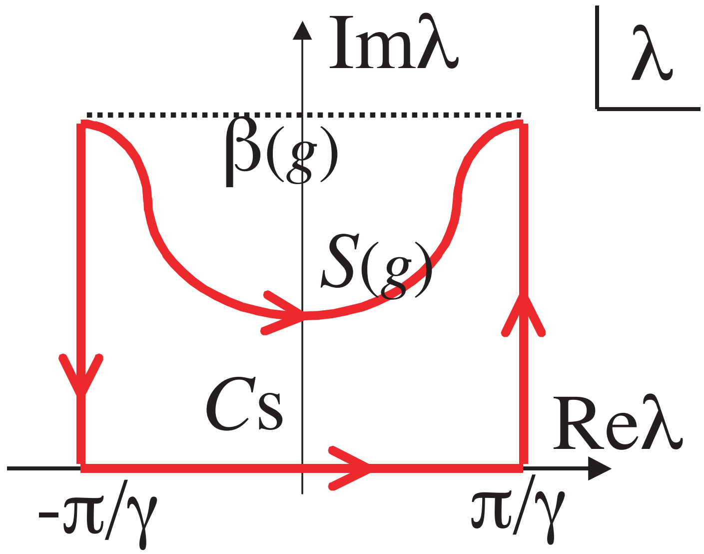


Figure 4.3: The loop $C_{\mathcal{S}}$ in the complex λ plane.

for $\lambda \in \mathcal{S}(g)$. The poles of the integrand in Eq. (4.31),

$$\frac{\gamma \sinh(2\gamma)}{\cosh(2\gamma) - \cos\{\gamma(\lambda - \Lambda)\}}$$

in the Λ plane are located at $\Lambda = \lambda \pm 2\mathrm{i}$. They never appear in the area $C_{\mathcal{S}}$ shown in Fig. 4.3 as long as $-1 < \mathrm{Im}\,\lambda < 1$ and $-1 < \mathrm{Im}\,\Lambda < 1$, where we denote the end points of $\mathcal{S}(g)$ by $\pm\pi/\gamma + \mathrm{i}\beta$.

When the imaginary part of the end points of the curve $\mathcal{S}(g)$, $\beta(g)$becomes $\beta(g) = 1$ as we increase the non-Hermiticity g, the left-hand side of Eq. (4.31) diverges and we expect that the system changes dramatically.

We obtain the non-Hermiticity g at which the end points of the curve $\mathcal{S}(g)$ reaches the points $\beta(g) = 1$. The quasimomenta with $\mathrm{Re}k = \pm\pi/\gamma$ may correspond to J_1 and J_M in Eq. (4.29) for $L \to \infty$. Hence we assume $z_{\mathcal{S}}(\lambda) = \pm 1/4$ for the end points of $\mathcal{S}(g)$. We thereby obtain the non-Hermiticity g by substituting $\pm 1/4$ for $z_{\mathcal{S}}(\lambda)$ and $\pm\pi/\gamma + \mathrm{i}$ for λ in Eq. (4.30). The result is equal to the non-Hermitian critical point g_{c} in Eq. (4.18) where the energy gap due to the spinon excitation vanishes.

As long as g is less than g_{c}, we can modify the integral contour as

$$\int_{\mathcal{S}(g)} = \int_{-\pi/\gamma+\mathrm{i}\beta(g)}^{-\pi/\gamma} + \int_{-\pi/\gamma}^{\pi/\gamma} + \int_{\pi/\gamma}^{\pi/\gamma+\mathrm{i}\beta(g)}, \tag{4.32}$$

where we assume that the expression of the distribution function $\sigma(\lambda)$ defined on the curve $\mathcal{S}(g)$ is valid everywhere within the area $C_{\mathcal{S}}$ as shown in Fig. 4.3. We thus rewrite Eq. (4.31) in the form

$$\frac{\gamma \sinh\gamma}{\cosh\gamma - \cos\gamma\lambda} = 2\pi\sigma(\lambda) + \int_{-\pi/\gamma}^{\pi/\gamma} \frac{\gamma \sinh(2\gamma)}{\cosh(2\gamma) - \cos\{\gamma(\lambda - \Lambda)\}} \sigma(\Lambda) d\Lambda. \tag{4.33}$$

We solve Eq. (4.33) by considering Fourier transformation and obtain $\sigma(\lambda)$ of the form

$$\sigma(\lambda) = \sum_{n=-\infty}^{n=\infty} \frac{e^{-in\gamma\lambda}}{2\cosh(n\gamma)}, \tag{4.34}$$

because the integrand in Eq. (4.31) has the periodicity $2\pi/\gamma$,. The distribution function $\sigma(\lambda)$ in Eq. (4.34) has the same expression as in the Hermitian case in Eq. (4.3); it suggests that the analytic continuation of the solution $\sigma(\lambda)$ in Eq. (4.34) may be valid inside the area $C_{\mathcal{S}}(g_c)$, where $C_{\mathcal{S}}(g_c)$ is the area $C_{\mathcal{S}}$ at $g = g_c$.

Eigenenergies

We calculate the dependence of eigenenergies, specifically, the ground-state energy and the spinon excitation energy on the non-Hermiticity g for $g < g_c$.

We first obtain the ground state energy E_{gs}. The ground-state energy E_{gs} per site is

$$E_{gs} = \frac{J}{L}\sum_{j=1}^{M}(\cos k_j - \Delta) + \frac{\Delta J}{4} = -\frac{J}{L}\sum_{j=1}^{M} \frac{\sinh^2\gamma}{\cosh\gamma - \cos\gamma\lambda_j} + \frac{\Delta J}{4}. \tag{4.35}$$

In the thermodynamic limit for $L \to \infty$ under $M/L = 1/2$, we have

$$E_{gs} = -J\int_{\mathcal{S}(g)} \frac{\sinh^2\gamma}{\cosh\gamma - \cos\gamma\lambda}\sigma(\lambda)d\lambda + \frac{\Delta J}{4}, \tag{4.36}$$

where $\sigma(\lambda)$ denotes the distribution function of the spin rapidity λ in Eq. (4.34). As long as there are no poles in $C_{\mathcal{S}}$, that is, g is less than g_c, we can modify the integral counter $\int_{\mathcal{S}}$ as $\int_{-\pi/\gamma}^{\pi/\gamma}$. The ground-state energy E_{gs} becomes

$$\begin{aligned} E_{gs} &= -\int_{-\pi/\gamma}^{\pi/\gamma} \frac{\sinh^2\gamma}{\cosh\gamma - \cos\gamma\lambda}\sigma(\lambda)d\lambda + \frac{\Delta J}{4} \\ &= -J\sinh\gamma\left[\frac{1}{2} + 2\sum_{n=1}^{\infty}\frac{1}{e^{2n\gamma}+1}\right] + \frac{\Delta J}{4}, \end{aligned} \tag{4.37}$$

which does not depend on g for $g < g_c$.

We next obtain the excitation energy $\mathcal{E}(\lambda_1, \lambda_2)$ of the two-spinon excitation. It also has the same expression as the Hermitian case in Eq. (4.2) after assuming that we can modify the integral counter $\int_{\mathcal{S}(g)}$ to $\int_{-\pi/\gamma}^{\pi/\gamma}$; the g dependence of the excitation energy appears in λ_1 and λ_2 on the distribution curve $\mathcal{S}(g)$, whose shape depends on g. The analytical continuation of the excitation $\mathcal{E}(\lambda_1, \lambda_2)$ is thus considered to be valid within the area $C_{\mathcal{S}}(g_c)$.

We now discuss how the energy gap Δ_{spinon} due to a pair of spinon excitations vanishes as we increase the non-Hermiticity g for $g < g_c$. In the non-Hermitian case, we define the energy gap Δ_{spinon} as the excitation energy $\mathcal{E}(\lambda_1, \lambda_2)$ at $\lambda_1 = \pm\pi/\gamma + i\beta(g)$ and at $\lambda_2 = \pm\pi/\gamma + i\beta(g)$ on the curve $\mathcal{S}(g)$. We first obtain the dependence of $p(\lambda)$ in Eq. (4.8) on β of the form

$$p(\lambda = \pm\pi/\gamma + i\beta) = \pm\frac{\pi}{2} + i\frac{\gamma\beta}{2} + i\sum_{n=1}^{\infty}\frac{(-1)^n\sinh(n\gamma\beta)}{n\cosh(n\gamma)} \tag{4.38}$$

by substituting $\lambda = \pm\pi/\gamma + i\beta$ into Eq. (4.8). We next obtain the dependence of g on β. In order to make the above discussion easy, we consider the following expansions of $\theta_1(\lambda)$ and $\theta_2(\lambda)$ in Eq. (4.30):

$$\theta_1(\lambda) = \gamma\lambda + \mathrm{i}\sum_{n\neq 0}\frac{\exp(-\mathrm{i}n\gamma\lambda - \gamma|n|)}{n},$$
$$\theta_2(\lambda) = \gamma\lambda + \mathrm{i}\sum_{n\neq 0}\frac{\exp(-\mathrm{i}n\gamma\lambda - 2\gamma|n|)}{n}. \tag{4.39}$$

By substituting Eqs. (4.34) and (4.39) into Eq. (4.30), we have

$$2g = 2\pi\mathrm{i}z_{\mathcal{S}}(\lambda) - \mathrm{i}\frac{\gamma\lambda}{2} + \sum_{n\neq 0}\frac{e^{-\mathrm{i}n\gamma\lambda}}{2n\cosh(n\gamma)} + \frac{\gamma\beta}{2} + \sum_{n=1}^{\infty}\frac{(-1)^n\sinh(n\gamma\beta)}{n\cosh(n\gamma)}. \tag{4.40}$$

By substituting $\lambda = \pm\pi/\gamma + \mathrm{i}\beta$ into Eq. (4.40), we then have

$$\begin{aligned}2g =& 2\pi\mathrm{i}z_{\mathcal{S}}(\pm\pi/\gamma + \mathrm{i}\beta) - \mathrm{i}\frac{\gamma}{2}\left(\pm\frac{\pi}{\gamma} + \mathrm{i}\beta\right) + \frac{\gamma\beta}{2} + 2\sum_{n=1}^{\infty}\frac{(-1)^n\sinh(n\gamma\beta)}{n\cosh(n\gamma)}\\ =& \gamma\beta + 2\sum_{n=1}^{\infty}\frac{(-1)^n\sinh(n\gamma\beta)}{n\cosh(n\gamma)},\end{aligned} \tag{4.41}$$

since

$$z_{\mathcal{S}}(\pm\pi/\gamma + \mathrm{i}\beta) = \frac{\pm(L/2-1)/2}{L} \to \pm\frac{1}{4} \tag{4.42}$$

as $L \to \infty$. We thus obtain the dependence of the non-Hermiticity g on β of the form

$$g = \frac{\gamma\beta}{2} + \sum_{n=1}^{\infty}\frac{(-1)^n\sinh(n\gamma\beta)}{n\cosh(n\gamma)}. \tag{4.43}$$

By considering Eqs. (4.38) and (4.43), we thus obtain the dependence of p on g of the form

$$p = \pm\frac{\pi}{2} + ig. \tag{4.44}$$

We thus obtain the explicit relation between Δ_{spinon} and g of the form

$$\begin{aligned}\Delta_{\mathrm{spinon}} &= \frac{JK(u)\sinh\gamma}{\pi}\left[\sqrt{1 - u^2\sin^2\left(\pm\frac{\pi}{2} + ig\right)} + \sqrt{1 - u^2\sin^2\left(\pm\frac{\pi}{2} + ig\right)}\right]\\ &= \frac{2JK(u)\sinh\gamma}{\pi}\sqrt{1 - u^2\cosh^2 g}\end{aligned} \tag{4.45}$$

by substituting $p(\lambda_1) = \pm\frac{\pi}{2} + ig$ and $p(\lambda_1) = \pm\frac{\pi}{2} + ig$ into Eq. (4.9). Figure 4.4 shows the g dependence of the energy gap Δ_{spinon} due to the spinon excitation for $\gamma = 3.5$.

We here comment that the energy gap Δ_{spinon} has a singularity at $g = g_{\mathrm{c}}(= \mathrm{arccosh}(1/u))$ with the exponent 1/2. We consider the Taylor expansion for Δ_{spinon} around $g = g_{\mathrm{c}}$ in the form

$$\Delta_{\mathrm{spinon}} \simeq \frac{8JK(u)\sinh\gamma}{\pi}(1-u^2)^{1/4}(g_{\mathrm{c}} - g)^{1/2} + \mathrm{O}(g_{\mathrm{c}} - g). \tag{4.46}$$

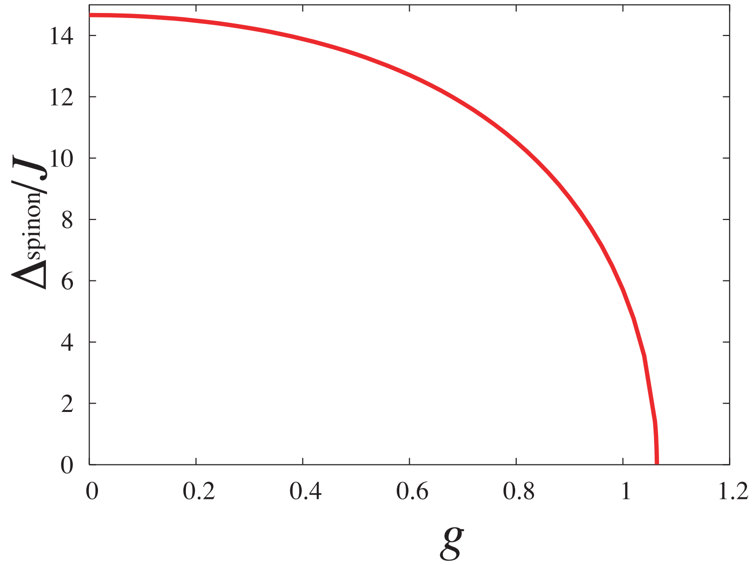


Figure 4.4: The g dependence of the energy gap Δ_{spinon} due to the two-spinon excitation for the antiferromagnetic non-Hermitian *XXZ* chain with $\gamma = 3.5$. The non-Hermitian critical point is $g_{\mathrm{c}} \cong 1.05867$.

Its exponent $1/2$ is the same for the Hubbard model in the half-filled case.

For $g \geq g_{\mathrm{c}}$, on the other hand, Albertini *et al.* [16] showed that the shape of the distribution curve $\mathcal{S}(g)$ is quite different from the one for $g < g_{\mathrm{c}}$. The Bethe-ansatz equation thus does not become the Hermitian one at all. It is therefore difficult to know ground-state properties of the non-Hermitian *XXZ* chain (4.15) for $g \geq g_{\mathrm{c}}$. However, we expect that the ground-state energy becomes complex in the region $g > g_{\mathrm{c}}$ on the basis of finite-size data shown in §6.2.

4.2.2 Physical meaning of the non-Hermitian generalization

We argue physical meaning of the non-Hermitian generalization of the *XXZ* chain (4.15); the non-Hermiticity g makes the dispersion relation $\mathcal{E}(p_s)$ of a spinon transformed to $\mathcal{E}(p_s + ig)$.

For the non-Hermitian *XXZ* chain (4.15), let us first obtain the momentum $p_s(g)$ of the spinon at the rapidity λ_s, or, at the quantum number J_s in Eq. (4.29) defined as

$$p_s(g) \equiv \sum_{\alpha=1}^{M} k_\alpha^{(\mathrm{gs})} - \sum_{\alpha=1}^{M-1} k_\alpha^{(\mathrm{es})} = \frac{2\pi J_s}{L} = 2\pi z_{\mathcal{S}}(\lambda_s), \tag{4.47}$$

where $\{k_\alpha^{(\mathrm{gs})}\}$ denotes the set of the quasimomenta for the ground state and $\{k_\alpha^{(\mathrm{es})}\}$ denotes the one for the excited state due to the spinon excitation at $\lambda_j^{\mathrm{gs}} = \lambda_s$; see the relation between k_j and λ_j in Eq. (4.26).

By taking Eqs. (4.8) and (4.43) into consideration, we rewrite Eq. (4.40) in the form

$$2g = 2\pi \mathrm{i} z_{\mathcal{S}}(\lambda_s) - ip(\lambda_s) + g, \tag{4.48}$$

or

$$g = \mathrm{i}p_s(g) - \mathrm{i}P_s, \tag{4.49}$$

where P_s denotes $p(\lambda_s)$. We assume that analytic continuation of the excitation energy $\mathcal{E}(\lambda_s)$, or $\mathcal{E}(p(\lambda_s)) = \mathcal{E}(P_s)$ is valid for $g < g_\mathrm{c}$ as discussed in §4.2.1. The excitation energy $\mathcal{E}(P_s)$ is then rewritten as $\mathcal{E}(p_s(g) + ig)$. Since $p_s(g)$ is real, we have the same structure as Eqs. (1.6) and (2.15). We may be thus able to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$ in the complex momentum p by analyzing the non-Hermitian Hamiltonian (4.15).

The assumption where the analytic continuation of the excitation energy at $\lambda = \lambda_s$ is valid everywhere inside the area $C_{\mathcal{S}}(g_\mathrm{c})$ in the complex rapidity space is thus equivalent to the assumption where the analytic continuation of the dispersion relation is valid in the area $\mathrm{Im}\, p < g_\mathrm{c}$ in the complex momentum space. Now that we consider the two-spinon excitation, the analytic continuation may be valid in the region

$$\mathrm{Im}\, p_\mathrm{spinon} < 2g_\mathrm{c}. \tag{4.50}$$

The zeros in Eq. (4.14) in the complex momentum space indeed exist in the area $\mathrm{Im}\, p_\mathrm{spinon} < 2g_\mathrm{c}$.

Chapter 5

Majumdar-Ghosh model

In the previous discussions for exactly solved strongly correlated quantum systems in Chapters 2, 3 and 4, we revealed that the imaginary part of a zero of the dispersion relation is equal to the inverse or twice the inverse correlation length. We then used the non-Hermitian systems in order to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$. We expect that we can develop the parallel discussions for unsolved models. In this chapter, we discuss the Majumdar-Ghosh model under the periodic boundary condition [17, 18]

$$\mathcal{H}_{\mathrm{MG}} = J\sum_{l=1}^{L}[\frac{1}{2}(S_{l+1}^{+}S_{l}^{-} + S_{l}^{+}S_{l+1}^{-}) + S_{l}^{z}S_{l+1}^{z}] + \frac{J}{2}\sum_{l=1}^{L}[\frac{1}{2}(S_{l+2}^{+}S_{l}^{-} + S_{l}^{+}S_{l+2}^{-}) + S_{l}^{z}S_{l+2}^{z}] \tag{5.1}$$

for $J > 0$ in the antiferromagnetic region. The Hamiltonian (5.1) has two-fold degenerate ground states and has a finite energy gap [19]. However, only variational estimates of the energy gap are known [20, 21]. We reveal in §5.2 that the imaginary part of a zero of the **variational** dispersion relation of the two-particle excitation is equal to twice the inverse correlation length. We calculate the correlation length from finite-size scaling of the correlation function of the ground state in §5.1. In §5.3, we propose a non-Hermitian Hamiltonian of the Majumdar-Ghosh model in order to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$.

5.1 Correlation length of the Majumdar-Ghosh model

Let us first calculate the correlation length of the Majumdar-Ghosh model from finite-size scaling of the correlation function of the ground state. The two-fold degenerate ground states of the Majumdar-Ghosh model (5.1) are

$$\begin{aligned} |\Psi_{\mathrm{gs}}\rangle_{+} &= \frac{1}{\sqrt{2 + 4\cdot 2^{-L/2}}}(|\Phi_{\mathrm{I}}\rangle + |\Phi_{\mathrm{II}}\rangle), \\ |\Psi_{\mathrm{gs}}\rangle_{-} &= \frac{1}{\sqrt{2 - 4\cdot 2^{-L/2}}}(|\Phi_{\mathrm{I}}\rangle - |\Phi_{\mathrm{II}}\rangle), \end{aligned} \tag{5.2}$$

where the wave functions $|\Phi_{\rm I}\rangle$ and $|\Phi_{\rm II}\rangle$ are defined by

$$\begin{aligned}|\Phi_{\rm I}\rangle &= |\phi_{1,2}\rangle \otimes |\phi_{3,4}\rangle \otimes \cdots \otimes |\phi_{L-1,L}\rangle,\\ |\Phi_{\rm II}\rangle &= |\phi_{2,3}\rangle \otimes |\phi_{4,5}\rangle \otimes \cdots \otimes |\phi_{L,1}\rangle\end{aligned} \tag{5.3}$$

with $|\phi_{i,j}\rangle$ denoting the singlet state of a pair of spins at sites i and j:

$$|\phi_{i,j}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle).$$

Note that $|\Phi_{\rm I}\rangle$ and $|\Phi_{\rm II}\rangle$ are not orthogonal for finite L: $\langle\Phi_{\rm I}|\Phi_{\rm II}\rangle = \langle\Phi_{\rm II}|\Phi_{\rm I}\rangle = 2^{-L/2+1}$. The states (5.2), on the other hand, are orthonormal.

The correlation functions $\langle S_0^z S_r^z\rangle = {}_\pm\langle\Psi_{\rm gs}|S_0^z S_r^z|\Psi_{\rm gs}\rangle_\pm$ with respect to the two-fold degenerate ground states $|\Psi_+\rangle$ and $|\Psi_-\rangle$ of the system of size L are given by

$$\begin{aligned}4\langle S_0^z S_1^z\rangle_\pm &= \frac{-1 \mp 2^{-L/2+2}}{2 \pm 2^{-L/2+2}}\\ &= -\frac{1}{2} \mp 2^{-L/2} + \mathrm{O}\left((2^{-L/2})^2\right),\\ 4\langle S_0^z S_{2i}^z\rangle_\pm &= \frac{\pm 2^{-L/2+1}}{1 \pm 2^{-L/2+1}}\\ &= \pm 2^{-L/2+1} + \mathrm{O}\left((2^{-L/2})^2\right) \qquad (\text{for } i \geq 1),\\ 4\langle S_0^z S_{2i+1}^z\rangle_\pm &= \frac{\mp 2^{-L/2+1}}{1 \pm 2^{-L/2+1}}\\ &= \mp 2^{-L/2+1} + \mathrm{O}\left((2^{-L/2})^2\right) \qquad (\text{for } i \geq 1).\end{aligned} \tag{5.4}$$

Assuming finite-size correction of the correlation function in the form

$$\langle S_0^z S_r^z\rangle_L = \langle S_0^z S_r^z\rangle_\infty + \mathrm{O}\left(\exp(-L/\xi)\right), \tag{5.5}$$

we obtain the correlation length

$$\xi = \frac{2}{\ln 2}. \tag{5.6}$$

5.2 Zeros of the dispersion relation and the correlation length

In this section, we use a variational approach to argue that the imaginary part of zeros in the complex momentum space of the dispersion relation of the spinon excitation may be equal to *twice* the inverse correlation length. As mentioned for the antiferromagnetic *XXZ* chain in §4.1, the factor *two* comes from the fact that the first excited state involves two spinons.

Although the exact dispersion relation is not obtained, some variational forms are obtained. The dispersion relation was first obtained by Shastry and Sutherland [20] with a trial wave function and then by Caspers *et al.* [21] with a variational wave function. The dispersion relation of the Hermitian Majumdar-Ghosh model given by Shastry and Sutherland [20] is

$$\epsilon_{\rm S}(p) = J\left(\frac{5}{4} + \cos p\right), \tag{5.7}$$

where p is a momentum of the spinon. All zeros $p_{\rm S}^{(0)}$ of the dispersion relation (5.7) in the region $\mathrm{Im}\, p \geq 0$ are

$$p_{\rm S}^{(0)} = \pm\pi + \mathrm{i} \ln 2. \tag{5.8}$$

The variational form of the dispersion relation given by Caspers *et al.* [21] is

$$\epsilon_{\rm C}(p) = \frac{(60r+34)\cos 2p - (278r+340)\cos p - (475r-731)}{(16r+8)\cos 2p - (56r+140)\cos p - (104r-172)} J \tag{5.9}$$

with

$$r = \frac{\sqrt{2\cos 2p - 20\cos p + 43}}{5 + 4\cos p}. \tag{5.10}$$

All zeros $p_{\rm C}^{(0)}$ of the dispersion relation (5.9) in the region $\mathrm{Im}\, p \geq 0$ are

$$p_{\rm C}^{(0)} = \pm\pi + \mathrm{i} \ln 2 \tag{5.11}$$

and

$$p_{\rm C}^{(0)} = \arccos\left(\frac{5}{2} - 2\mathrm{i}\right) \simeq (0.80\ldots) + \mathrm{i}(1.85\ldots). \tag{5.12}$$

In both cases, the imaginary part of the zeros in Eq. (5.8) and the zeros nearest to the real axis in Eq. (5.11) is equal to *twice* the inverse correlation length of the spinon excitation.

5.3 Non-Hermitian analysis of the Majumdar-Ghosh model

In order to obtain the dispersion relation on the axis $\mathrm{Im}\, p = g$ in the complex momentum space, we consider the non-Hermitian generalization of the Majumdar-Ghosh model. In analogy to the non-Hermitian generalization of the antiferromagnetic XXZ chain discussed in §4.2, we analyze the non-Hermitian Hamiltonian:

$$\begin{aligned}\mathcal{H}_{\rm MG}(g) =& J\sum_{l=1}^{L}[\frac{1}{2}(e^{2g}S_{l+1}^{+}S_{l}^{-} + e^{-2g}S_{l}^{+}S_{l+1}^{-}) + S_{l}^{z}S_{l+1}^{z}] \\ &+ \frac{J}{2}\sum_{l=1}^{L}[\frac{1}{2}(e^{4g}S_{l+2}^{+}S_{l}^{-} + e^{-4g}S_{l}^{+}S_{l+2}^{-}) + S_{l}^{z}S_{l+2}^{z}].\end{aligned} \tag{5.13}$$

The above Hamiltonian can be derived from the effective Hamiltonian of the non-Hermitian t-t'-U model in the half-filled case as shown in Appendix E:

$$\begin{aligned}\mathcal{H}_{t\text{-}t'\text{-}U}(g) = &-t\sum_{l=1}^{L}(e^{g}c_{l+1,\uparrow}^{\dagger}c_{l,\uparrow} + e^{-g}c_{l,\uparrow}^{\dagger}c_{l+1,\uparrow} + e^{-g}c_{l+1,\downarrow}^{\dagger}c_{l,\downarrow} + e^{g}c_{l,\downarrow}^{\dagger}c_{l+1,\downarrow}) \\ &- t'\sum_{l=1}^{L}(e^{2g}c_{l+2,\uparrow}^{\dagger}c_{l,\uparrow} + e^{-2g}c_{l,\uparrow}^{\dagger}c_{l+2,\uparrow} + e^{-2g}c_{l+2,\downarrow}^{\dagger}c_{l,\downarrow} + e^{2g}c_{l,\downarrow}^{\dagger}c_{l+2,\downarrow}) + U\sum_{l=1}^{L}n_{l,\uparrow}n_{l,\downarrow},\end{aligned} \tag{5.14}$$

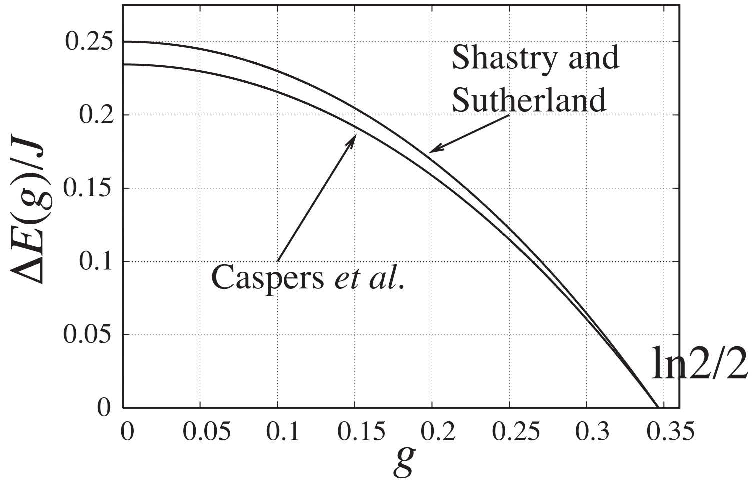


Figure 5.1: The non-Hermiticity dependence of the approximate estimates of the energy gap calculated by Shastry and Sutherland's approach and by Caspers *et al.*'s approach.

with $J \equiv 4t^2/U$ and $J/2 \equiv 4t'^2/U$ in Eq. (5.13).

We calculate the non-Hermitian critical point g_c where approximate estimates of the energy gap vanish. For both dispersion relations obtained by Shastry and Sutherland in Eq. (5.7) and by Caspers *et al.* in Eq. (5.9), the excitation energy at $p = \pm\pi$ determines the energy gaps. For the non-Hermitian Majumdar-Ghosh model (5.13), we assume that the non-Hermiticity g shifts the momentum k of one defect by $\mathrm{i}g$. Since we consider a two-spinon excitation, we replace the momentum p in Eq. (5.7) and in Eq. (5.9) by $p + 2\mathrm{i}g$. We below argue that the non-Hermitian critical point g_c where the energy gap vanishes is equal to the inverse correlation length $1/\xi = \ln 2/2$; it suggests that the non-Hermitian Hamiltonian (5.13) can yield the dispersion relation on the axis $\mathrm{Im}\, p = g$. We thereby assume that the energy gap $\Delta E(g)$ is given by the excitation energy $\epsilon(\pm\pi + 2ig)$.

The dependence of the energy gap $\Delta E_\mathrm{S}(g)$ on the non-Hermiticity g on the basis of $\epsilon_\mathrm{S}(p)$ in Eq. (5.7) is thus given by

$$\Delta E_\mathrm{S}(g) = \epsilon_\mathrm{S}(\pm\pi + 2\mathrm{i}g) = J\left(\frac{5}{4} - \cosh(2g)\right). \tag{5.15}$$

As shown in Fig. 5.1, the non-Hermitian critical point g_c where the energy gap $\Delta E_\mathrm{S}(g)$ vanishes is $g_c = \ln 2/2$. The dependence of the energy gap $\Delta E_\mathrm{C}(g)$ on the non-Hermiticity g on the basis of $\epsilon_\mathrm{C}(p)$ in Eq. (5.9) is again given by

$$\begin{aligned}\Delta E_\mathrm{C}(g) &= \epsilon_\mathrm{C}(\pm\pi + 2\mathrm{i}g)\\ &= \frac{(60R+34)\cosh(4g) + (278R+340)\cosh(2g) - (475R-731)}{(16R+8)\cosh(4g) + (56R+80)\cosh(2g) - (104R-172)}J\end{aligned} \tag{5.16}$$

with

$$R = \sqrt{\frac{2\cosh(4g) + 20\cosh(2g) + 43}{(5-4\cosh(2g))^2}}. \tag{5.17}$$

As shown in Fig. 5.1, the non-Hermitian critical point g_c is $g_c = \ln 2/2$ again. In both cases, the non-Hermitian critical point g_c is equal to the inverse correlation length $\xi^{-1} = \ln 2/2$ in Eq. (5.6).

We now give a piece of evidence that the non-Hermitian critical point is exactly $g_c = \ln 2/2$ by showing that the ground-state property drastically changes at $g = \ln 2/2$. The non-Hermitian Majumdar-Ghosh model (5.13) has two-fold degenerate dimer ground states as in the Hermitian case. The right eigenfunctions $|\Psi^{\mathrm{R}}_{\pm}\rangle$ and the left eigenfunctions $\langle\Psi^{\mathrm{L}}_{\pm}|$ of the ground states of the system of size L are given by

$$\begin{aligned} |\Psi^{\mathrm{R}}_{\pm}\rangle &= \frac{1}{\sqrt{2 \pm 2\dfrac{e^{gL}+e^{-gL}}{2^{L/2}}}}\left(|\Phi^{\mathrm{R}}_{\mathrm{I}}\rangle \pm |\Phi^{\mathrm{R}}_{\mathrm{II}}\rangle\right), \\ \langle\Psi^{\mathrm{L}}_{\pm}| &= \frac{1}{\sqrt{2 \pm 2\dfrac{e^{gL}+e^{-gL}}{2^{L/2}}}}\left(\langle\Phi^{\mathrm{L}}_{\mathrm{I}}| \pm \langle\Phi^{\mathrm{L}}_{\mathrm{II}}|\right), \end{aligned} \tag{5.18}$$

where the wave functions $|\Phi^{\mathrm{R}}_{\mathrm{I,\,II}}\rangle$ and $\langle\Phi^{\mathrm{L}}_{\mathrm{I,\,II}}|$ are defined by

$$\begin{aligned} |\Phi^{\mathrm{R}}_{\mathrm{I}}\rangle &= |\phi^{\mathrm{R}}_{1,2}\rangle \otimes |\phi^{\mathrm{R}}_{3,4}\rangle \otimes \cdots \otimes |\phi^{\mathrm{R}}_{L-1,L}\rangle, \\ |\Phi^{\mathrm{R}}_{\mathrm{II}}\rangle &= |\phi^{\mathrm{R}}_{2,3}\rangle \otimes |\phi^{\mathrm{R}}_{4,5}\rangle \otimes \cdots \otimes |\phi^{\mathrm{R}}_{L,1}\rangle, \\ \langle\Phi^{\mathrm{L}}_{\mathrm{I}}| &= \langle\phi^{\mathrm{L}}_{1,2}| \otimes \langle\phi^{\mathrm{L}}_{3,4}| \otimes \cdots \otimes \langle\phi^{\mathrm{L}}_{L-1,L}|, \\ \langle\Phi^{\mathrm{L}}_{\mathrm{II}}| &= \langle\phi^{\mathrm{L}}_{2,3}| \otimes \langle\phi^{\mathrm{L}}_{4,5}| \otimes \cdots \otimes \langle\phi^{\mathrm{L}}_{L,1}| \end{aligned} \tag{5.19}$$

with $|\phi^{\mathrm{R}}_{i,j}\rangle$ and $\langle\phi^{\mathrm{L}}_{i,j}|$ denoting weighted singlet states of a pair of spins at sites i and j:

$$\begin{aligned} |\phi^{\mathrm{R}}_{i,j}\rangle &= \frac{1}{\sqrt{2}}\left(e^{-g}|\uparrow_i\downarrow_j\rangle - e^{g}|\downarrow_i\uparrow_j\rangle\right), \\ \langle\phi^{\mathrm{L}}_{i,j}| &= \frac{1}{\sqrt{2}}\left(e^{g}\langle\uparrow_i\downarrow_j| - e^{-g}\langle\downarrow_i\uparrow_j|\right). \end{aligned} \tag{5.20}$$

Equation (5.19) is consistent with Eq. (5.3) transformed by a many-body version of the imaginary gauge transformation [2]

$$\psi(x_1, x_2, \ldots; g) = \exp(g\sum_i x_i)\psi(x_1, x_2, \ldots; 0). \tag{5.21}$$

Note that $\langle\Phi^{\mathrm{L}}_{\mathrm{I}}|\Phi^{\mathrm{R}}_{\mathrm{I}}\rangle = \langle\Phi^{\mathrm{L}}_{\mathrm{II}}|\Phi^{\mathrm{R}}_{\mathrm{II}}\rangle = 1$ and $\langle\Phi^{\mathrm{L}}_{\mathrm{I}}|\Phi^{\mathrm{R}}_{\mathrm{II}}\rangle = \langle\Phi^{\mathrm{L}}_{\mathrm{II}}|\Phi^{\mathrm{R}}_{\mathrm{I}}\rangle = \left(e^{gL}+e^{-gL}\right)/2^{L/2}$, but $|\Psi^{\mathrm{R}}_{\pm}\rangle$ and $\langle\Psi^{\mathrm{L}}_{\pm}|$ are bi-orthonormal. We note that the ground-state energy $-\dfrac{3}{8}J$ per site does not depend on the non-Hermiticity g.

The correlation functions of the non-Hermitian system, $\langle S^z_0 S^z_r\rangle_{\pm} = \langle\Psi^{\mathrm{L}}_{\pm}|S^z_0 S^z_r|\Psi^{\mathrm{R}}_{\pm}\rangle$ with respect to the two-fold degenerate ground states $|\Psi^{\mathrm{R}}_{+}\rangle$ and $|\Psi^{\mathrm{R}}_{-}\rangle$ are obtained

(a) (b)

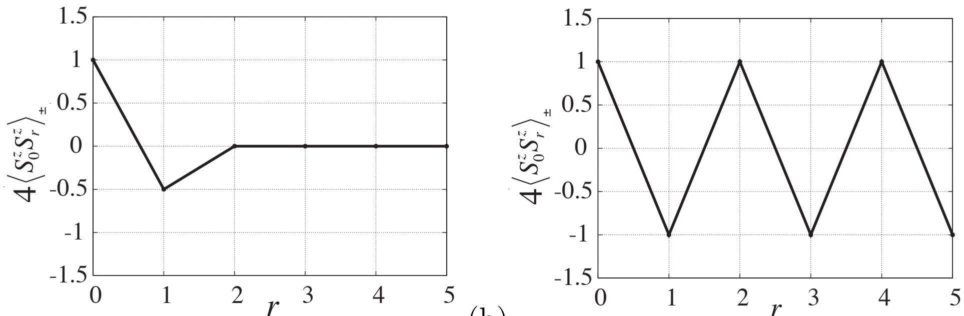


Figure 5.2: The correlation function $\langle S_0^z S_r^z \rangle_\pm$ of the non-Hermitian Majumdar-Ghosh model of infinite size in the regions (a) $g < \ln 2/2$ and (b) $g > \ln 2/2$.

in the forms

$$4\langle S_0^z S_1^z \rangle_\pm = \frac{-1 \mp 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}}{2 \pm 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}},$$

$$4\langle S_0^z S_{2i}^z \rangle_\pm = \frac{\pm 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}}{2 \pm 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}} \qquad (\text{for } i \geq 1),$$

$$4\langle S_0^z S_{2i+1}^z \rangle_\pm = \frac{\mp 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}}{2 \pm 2\dfrac{e^{gL} + e^{-gL}}{2^{L/2}}} \qquad (\text{for } i \geq 1). \tag{5.22}$$

Figure 5.2 shows the correlation function in the limit $L \to \infty$ in the region $0 < g < \ln 2/2$ and in the region $g > \ln 2/2$, respectively. The ground state is dimerized in the region $0 < g < \ln 2/2$ and is an extended state in the region $g > \ln 2/2$. The phase transition from the dimer state to the extended state reminds us of the localization-delocalization transition of the non-Hermitian random Anderson model discussed by Hatano and Nelson [2] (see Appendix A). The phase transition point $g_c = \ln 2/2$ then may be naturally regarded as the non-Hermitian critical point. We thus conjecture from the above discussions that the non-Hermitian critical point is equal to the inverse correlation length of the Hermitian systems for the Majumdar-Ghosh model.

Chapter 6

Numerical analysis of non-Hermitian models

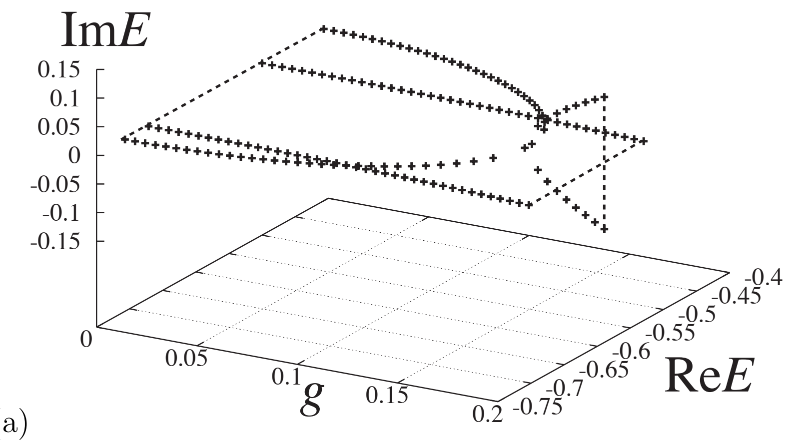
In the previous chapter, we discussed the non-Hermitian generalization of exactly solved models and suggested the conjecture that the non-Hermitian critical point g_{c} where the energy gap vanishes is equal to the inverse correlation length of the Hermitian system. We now numerically show that the inverse correlation length is consistent with the extrapolated estimate $g_{\mathrm{c}}(\infty)$ of finite-size data $g_{\mathrm{c}}(L)$ where an eigenvalue which corresponds to the ground state in the limit $L \to \infty$, becomes complex. We show the above for the Hubbard model in § 6.1, for the $S = 1/2$ XXZ chain in § 6.2 and for a frustrated quantum spin chain in § 6.3. Although we do not know the correlation length of the $S = 1/2$ antiferromagnetic Heisenberg chain with nearest- and next-nearest-neighbor interactions, we show in § 6.3 that the numerical estimate $g_{\mathrm{c}}(\infty)$ is consistent with the ground-state phase diagram.

6.1 Non-Hermitian Hubbard model

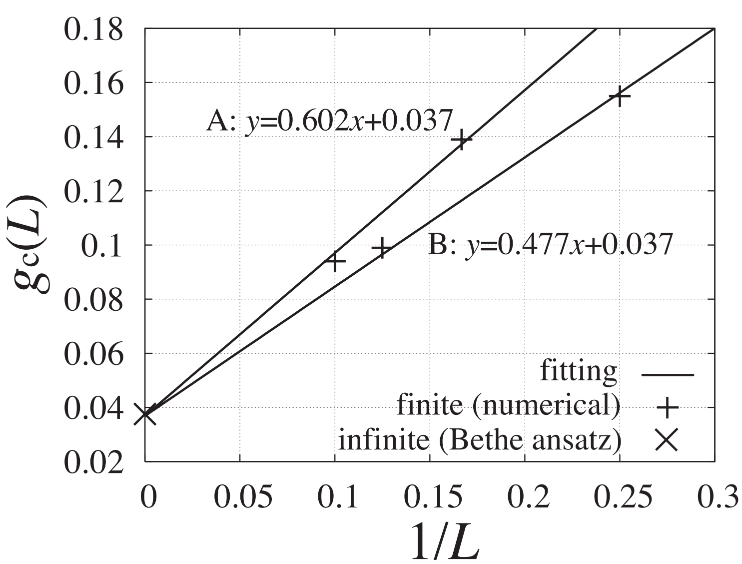
We first analyze the non-Hermitian Hubbard models (3.11) and (4.16) of size L. We define the non-Hermitian "critical" point $g_{\mathrm{c}}(L)$ of a finite system as the point where the energy gap between the ground state and a low-lying excited state vanishes and beyond which the ground-state energy becomes complex. We here show that the extrapolated estimate $g_{\mathrm{c}}(\infty)$ of finite-size data $g_{\mathrm{c}}(L)$ is close to the exact value of the correlation length.

We first use the non-Hermitian generalization of the form (3.11) in the subspace $S^z_{\mathrm{tot}} = 0$, which eliminates the charge gap. All eigenvalues are real at the Hermitian point $g = 0$. Upon increasing g, a pair of eigenvalues move on the real axis. They spread into the complex space when g exceeds a value $g_{\mathrm{c}}(L)$.

Figure 6.1 (a) shows the spectral flow of the eigenvalues per site for $L = 4$ around the ground state for $U = 2t$. The eigenvalues of the ground state and the third excited state move toward each other on the real axis and spread into the complex space as soon as the two eigenvalues collide, which gives the non-Hermitian "critical" point $g_{\mathrm{c}}(L)$. The eigenvalues of the first and the second excited states scarcely move. The movement of the ground-state energy is presumably a finite-size effect; the ground-state energy does not change for $g < g_{\mathrm{c}}$ for the infinite system as



(a)



(b)

Figure 6.1: (a) The spectral flow of the eigenvalues per site around the ground state for $L = 4$ with $U/t = 2$ as we increase the non-Hermiticity g which eliminates the charge gap. (b) The $1/L$ plot of $g_{\rm c}(L)$.

shown in Fig. 3.5.

We numerically estimated $g_{\rm c}(L)$ for $L = 4, 6, 8$ and 10 and extrapolated them to $g_{\rm c}(\infty)$ by considering the finite-size correction as follows:

$$g_{\rm c}(L) = g_{\rm c}(\infty) + a/L + {\rm O}(1/L^2). \tag{6.1}$$

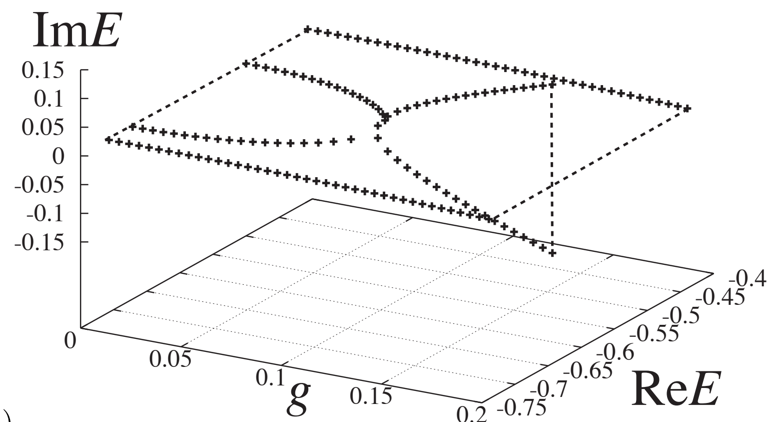
Figure 6.1 (b) shows the $1/L$ plot of $g_{\rm c}(L)$; this implies that we have to consider different finite-size corrections in the case $L = 4n$ (for $L = 4$ and 8) and in the case $L = 4n + 2$ (for $L = 6$ and 10). The reason why we have to consider different finite-size corrections is that the quantum numbers I_j and J_α in the Bethe-ansatz equations (3.17) and (3.18) are different between two cases; for $L = 4n+2$, we have $\{I_j\} = \{-(N-1)/2, \cdots, (N-1)/2\}$ and $\{J_\alpha\} = \{-(M-1)/2, \cdots, (M-1)/2\}$, whereas for $L = 4n$, we have $\{I_j\} = \{-N/2, \cdots, N/2-1\}$ and $\{J_\alpha\} = \{-(M-1)/2, \cdots, (M-1)/2\}$.

In Fig. 6.1 (b), the line A is the linear fitting of $g_{\rm c}(L)$ for $L = 6$ and 10 and the line B is that for $L = 4$ and 8; both lines are determined by the least-squares method under the condition that they have the same intercept $g_{\rm c}(\infty)$. The final estimate of $g_{\rm c}(\infty)$ is 0.037, while the Bethe-ansatz method yields $g_{\rm c} = 1/\xi_{\rm charge} \cong 0.038\ldots$. Our estimate is consistent with the exact value. It is quite remarkable to obtain such a good estimate from data for such small L.

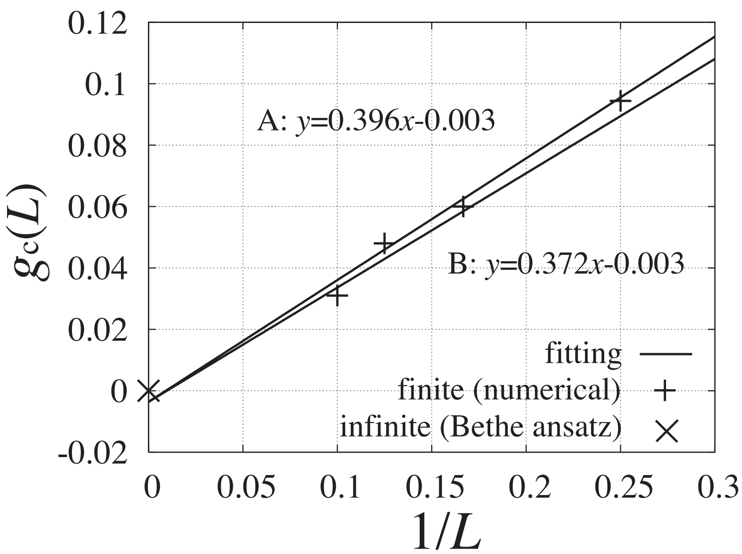
Figure 6.2 (a) shows the spectral flow for $L = 4$ around the ground state when we use the non-Hermitian generalization of the form (4.16), which eliminates the spin gap. The eigenvalues of the first and the second excited states move toward each other, while the eigenvalues of the ground state and the third excited state scarcely move. We presume that the energy gap between the ground state and the third excited state is caused by the charge excitation while the energy gap between the first and the second excited states is caused by the spinon excitation. We expect that the ground state and the first excited state are eventually degenerate in the thermodynamic limit. Hence we regard the collision of the first and second excited states as the ground-state transition. This behavior implies the charge-spin separation of one-dimensional quantum systems in the low-energy region [22]. Figure 6.2 (b) shows the $1/L$ plot of $g_{\rm c}(L)$. We obtain the extrapolated estimate $g_{\rm c}(\infty)$ by the same least-squares method as we used above; the line A shows the linear fitting of $g_{\rm c}(L)$ for $L = 4$ and 8 and the line B is that for $L = 6$ and 10, which yields the extrapolated estimate $g_{\rm c}(\infty) = -0.003$. Our estimate is also consistent with the exact value $g_{\rm c} = 1/\xi_{\rm spinon} = 0$.

6.2 Non-Hermitian $S = 1/2$ antiferromagnetic XXZ chain

We analyze the non-Hermitian $S = 1/2$ antiferromagnetic XXZ chain (4.15) in the Ising-like region $\Delta > 1$ for finite L. We numerically calculate the non-Hermitian "critical" point $g_{\rm c}(L)$ of the XXZ chain of size L. We obtain the extrapolated estimate $g_{\rm c}(\infty)$ of finite-size data $g_{\rm c}(L)$ and show that the estimate $g_{\rm c}(\infty)$ is consistent with the inverse correlation length of the Hermitian system. Figure 6.3 (a) shows the spectral flow per site around the ground state of the XXZ chain of $L = 8$ in

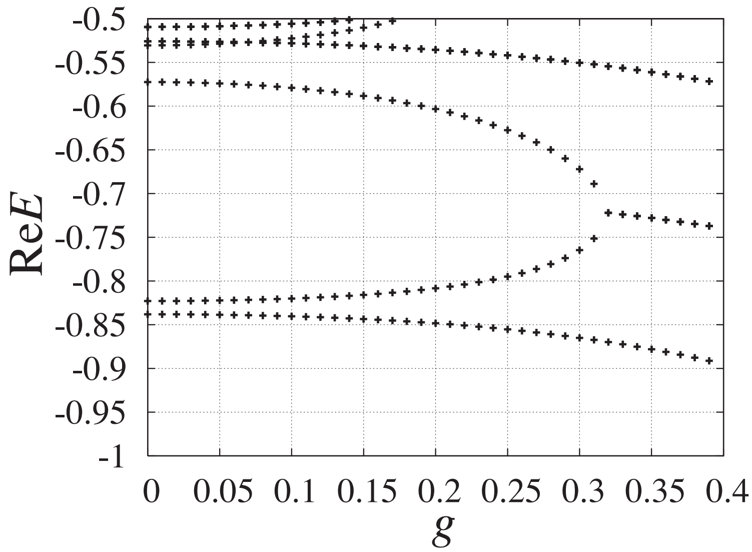


(a)

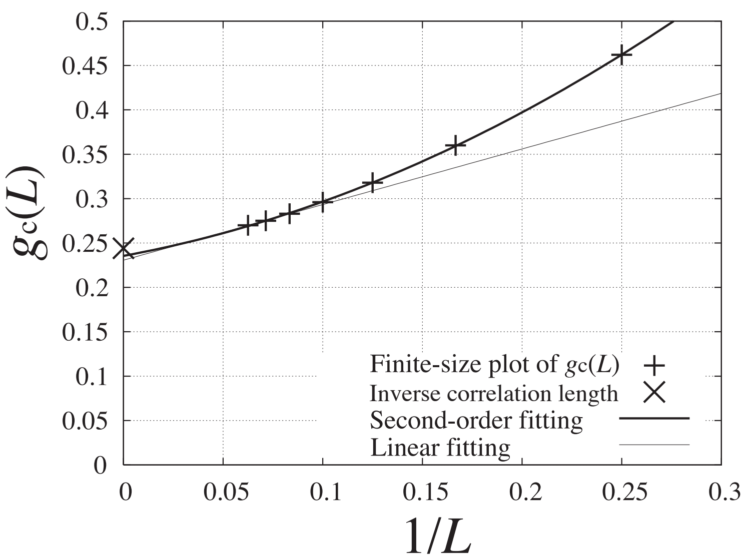


(b)

Figure 6.2: (a) The spectral flow of the eigenvalues per site around the ground state for $L = 4$ with $U/t = 2$ as we increase the non-Hermiticity g, which eliminates the spin gap. (b) The $1/L$ plot of $g_{\mathrm{c}}(L)$.



(a)



(b)

Figure 6.3: (a) The spectral flow of the eigenvalues per site of the XXZ chain for $L = 8$ with $\Delta = 3$. (b) The finite-size plot of $g_c(L)$ [4].

the subspace $S^z_{\mathrm{tot}} = 0$ as we increase the non-Hermiticity g for $\Delta = 3$. The pair of the first and the second excited states undergoes the real-complex transition, which is the same as in Fig. 6.2 (a). The ground state and the first excited state of Hermitian finite systems are eventually degenerate in the thermodynamic limit; the ground state has the Néel order in the region $\Delta > 1$ for infinite L. We therefore expect that the real-complex transition point of the first and second excited states converges to the non-Hermitian critical point g_{c} in the limit $L \to \infty$. We thereby use the real-complex transition point in order to define the non-Hermitian "critical" point $g_{\mathrm{c}}(L)$.

We then extrapolate the finite-size data. Figure 6.3 (b) shows the extrapolation of $g_{\mathrm{c}}(L)$ for the XXZ chain with $\Delta = 3$. The extrapolated estimate $g_{\mathrm{c}}(\infty)$ by linear fitting in the form

$$g_{\mathrm{c}}(L) = g_{\mathrm{c}}(\infty) + a/L + \mathrm{O}(1/L^2) \tag{6.2}$$

for $L = 12, 14$ and 16, is 0.231. In order to take the finite-size data $g_{\mathrm{c}}(L)$ for small L into consideration, we also calculate the extrapolated estimate $g_{\mathrm{c}}(\infty)$ by a second-order fitting in the form

$$g_{\mathrm{c}}(L) = g_{\mathrm{c}}(\infty) + a/L + b/L^2 + \mathrm{O}(1/L^3) \tag{6.3}$$

for $L = 4, 6, \ldots, 14, 16$ to obtain $g_{\mathrm{c}}(\infty) = 0.235$. Both estimates are consistent with the inverse correlation length $g_{\mathrm{c}} = 1/\xi \cong 0.244$ calculated analytically.

6.3 NNN Heisenberg chain

In this section, we consider the $S = 1/2$ antiferromagnetic Heisenberg chain with nearest- and next-nearest-neighbor interactions; we hereafter call this model the NNN Heisenberg chain. The Hermitian Hamiltonian of this model is

$$\mathcal{H}_{\mathrm{NNN}} = J \sum_{l=1}^{L} [\mathbf{S}_l \cdot \mathbf{S}_{l+1} + \alpha \mathbf{S}_l \cdot \mathbf{S}_{l+2}], \tag{6.4}$$

where $J > 0$ and $\alpha \geq 0$. We require the periodic boundary conditions. At the point $\alpha = 0$, the model is the standard Heisenberg chain. The ground state is a spin fluid state and the energy gap is zero. At the point $\alpha = 1/2$, the model is the Majumdar-Ghosh model [17, 18] and the energy gap is finite. Okamoto and Nomura [23] numerically showed that a massive-massless transition occurs at $\alpha_{\mathrm{c}} \cong 0.2411$.

We calculate the correlation length of the model (6.4). In general, it is hard to calculate the correlation length of the frustrated system (6.4) because the quantum Monte Carlo method is not efficient owing to the minus sign problem. By means of the density matrix renormalization group method, the correlation length are numerically obtained [15, 24]

In this section, we propose another method of obtaining the correlation length. The method is the non-Hermitian analysis of the NNN Heisenberg chain; specifically, we hereafter analyze the following Hamiltonian:

$$\begin{aligned}\mathcal{H}_{\rm NNN}(g) =& J\sum_{l=1}^{L}[\frac{1}{2}(e^{2g}S_{l+1}^{+}S_{l}^{-}+e^{-2g}S_{l}^{+}S_{l+1}^{-})+S_{l}^{z}S_{l+1}^{z}] \\ &+\alpha J\sum_{l=1}^{L}[\frac{1}{2}(e^{4g}S_{l+2}^{+}S_{l}^{-}+e^{-4g}S_{l}^{+}S_{l+2}^{-})+S_{l}^{z}S_{l+2}^{z}].\end{aligned} \tag{6.5}$$

We numerically estimated the non-Hermitian "critical" point $g_{\rm c}(L)$ of the system (6.5) of size L in the subspace $S_z^{\rm tot}=0$ where an eigenvalue which corresponds to the ground state in the thermodynamic limit becomes complex. We obtain the extrapolated estimate $g_{\rm c}(\infty)$ of finite-size data of $g_{\rm c}(L)$. We reveal that the estimate $g_{\rm c}(\infty)$ calculated from finite L systems is approximately consistent with the inverse correlation length.

Figure 6.4 shows the spectral flow of the eigenvalues per site around the ground state for $L=8$ with $\alpha=0.49$, $\alpha=0.5$ (the Majumdar-Ghosh point) and $\alpha=0.51$. In Fig. 6.4 (a) for $\alpha=0.49$, as we increase the non-Hermiticity g, the energy gap between the first excited state, which corresponds to one of the degenerate ground states in $L\to\infty$ [23], and the second excited state, which corresponds to the first excited state in $L\to\infty$, vanishes at $g=g_{\rm c1}(L)\cong 0.24$. These two eigenvalues become complex in the region $g_{\rm c1}(L)<g<g_{\rm c2}(L)$ before they become real again at $g=g_{\rm c2}(L)\cong 0.42$. We define the non-Hermitian "critical" point of a finite system for $\alpha<0.5$ as the point $g=g_{\rm c1}(L)$ where the first excited-state energy first becomes complex.

In Fig. 6.4 (b) for $\alpha=0.5$, the two-fold degenerate ground states exist for any g and the energy gap between the ground state and the first excited state vanishes at $g=g_{\rm c}(L)\cong 0.35$. However, these eigenvalues do not become complex for $g>g_{\rm c}(L)$. This is presumably because $g_{\rm c1}(L)=g_{\rm c2}(L)=g_{\rm c}(L)$. We still regard $g_{\rm c1}(L)$ as the non-Hermitian "critical" point $g_{\rm c}(L)$ for $\alpha=0.5$.

In Fig. 6.4 (c) for $\alpha=0.51$, the ground state and the first excited state never become complex for any g. The ground state for $\alpha>0.5$ is an incommensurate state of the spiral phase [25]. Our non-Hermitian generalization of the form (6.5) is presumably not appropriate for detecting the incommensurate state in the region $\alpha>0.5$ because we can never vanish the energy gap between two states which have the different wave numbers. In this region, other types of non-Hermitian generalization may be needed.

We hereafter restrict ourselves to the region $0\le\alpha\le 0.5$. We extrapolate the finite-size data $g_{\rm c}(L)$ for $L=4,8,12$ and 16 by the linear fitting in the form

$$g_{\rm c}(L)=g_{\rm c}(\infty)+a/L+{\rm O}(1/L^2) \tag{6.6}$$

and by the second-order fitting in the form

$$g_{\rm c}(L)=g_{\rm c}(\infty)+a/L+b/L^2+{\rm O}(1/L^3). \tag{6.7}$$

Figure 6.5 shows the extrapolated estimates $g_{\rm c}(\infty)$ in the region $0\le\alpha\le 0.5$. The second-order estimate $g_{\rm c}(\infty)$ around $\alpha\cong 0$ is almost zero and is consistent with $\xi^{-1}=0$ in the limit $L\to\infty$. The extrapolated estimates $g_{\rm c}(\infty)$ at $\alpha=0.5$ are

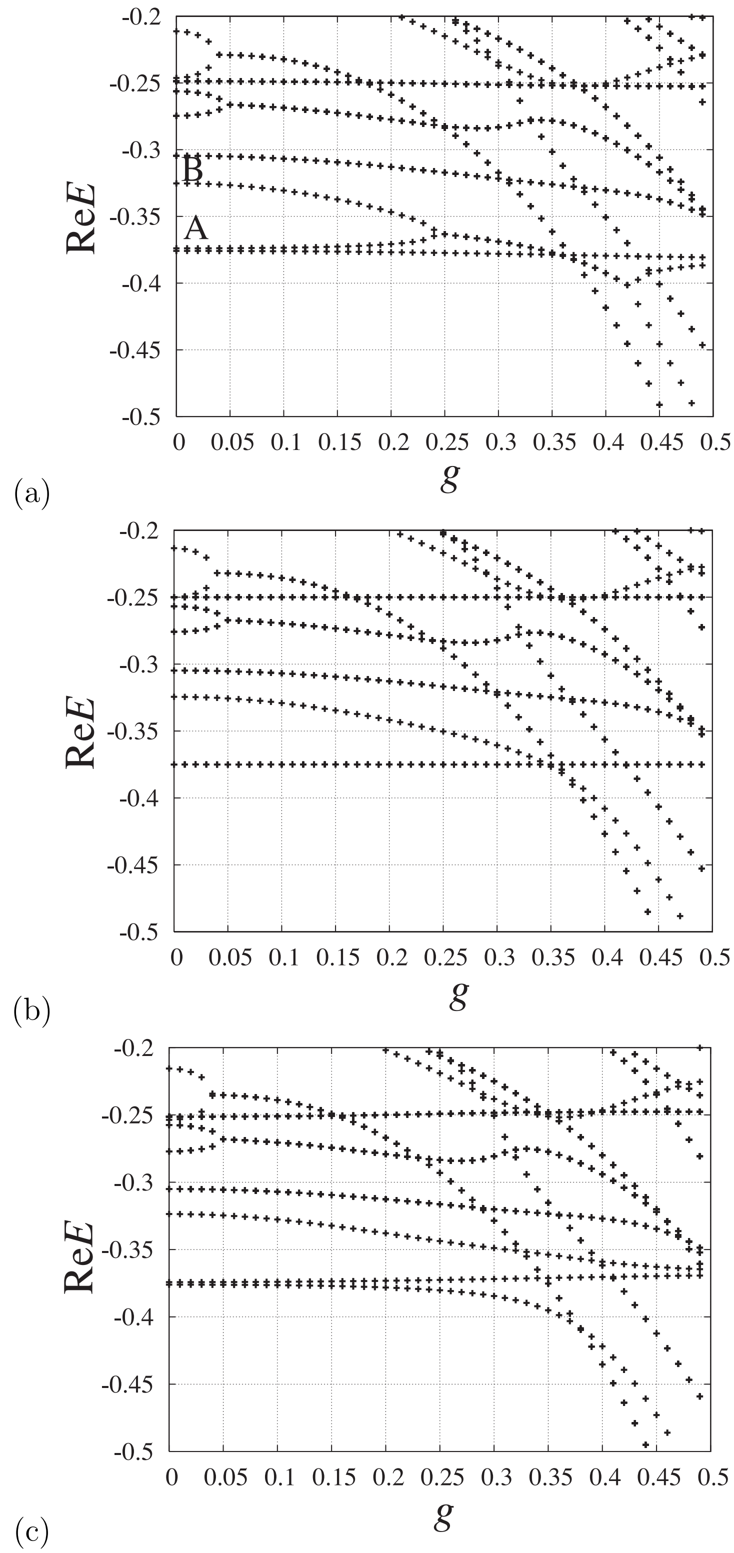


Figure 6.4: The spectral flow of the real part of the eigenvalues per site around the ground state for $L = 8$ with (a) $\alpha = 0.49$, (b) $\alpha = 0.5$ and (c) $\alpha = 0.51$.

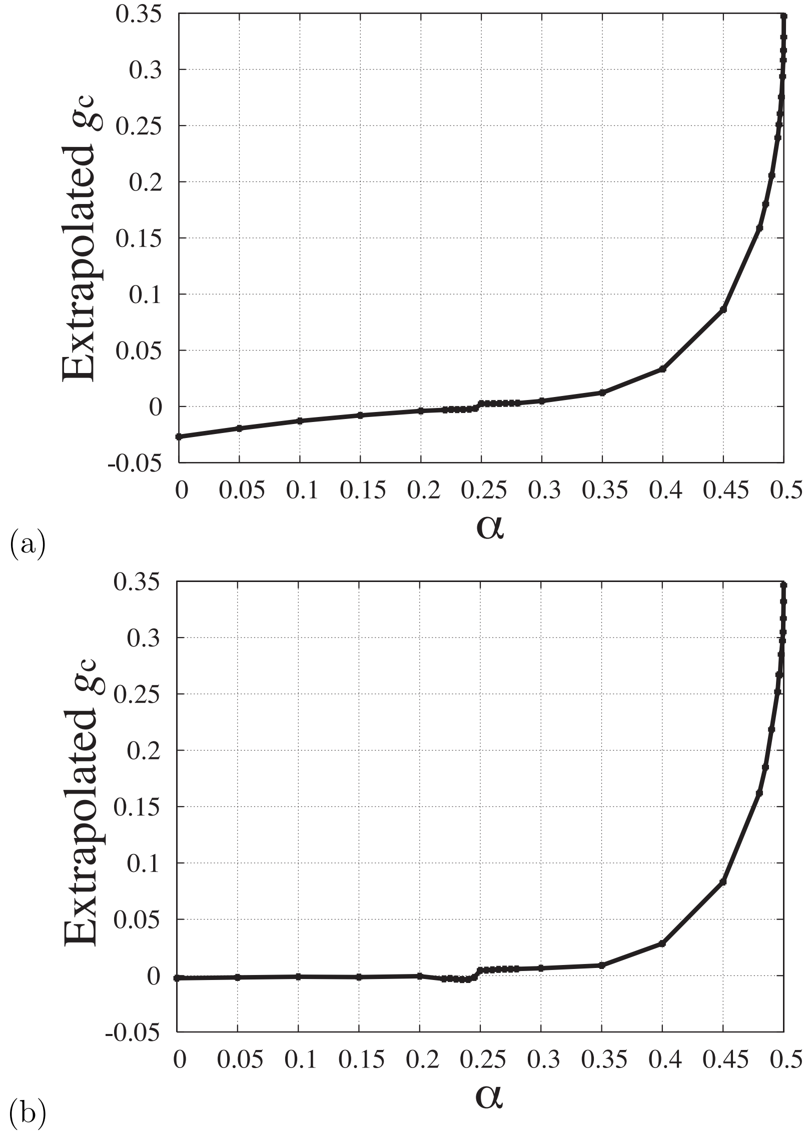


Figure 6.5: The extrapolated estimates $g_c(\infty)$ as a function of α in the region $0 \leq \alpha \leq 0.5$ by (a) a linear fitting and by (b) a second-order fitting.

around 0.35 for both linear and second-order fitting, which is consistent with the inverse correlation length $\xi^{-1} = \ln 2/2$ $(= 0.347\ldots)$; see § 5.1. At $\alpha = 0.48$, on the other hand, the extrapolated estimates $g_{\mathrm{c}}(\infty)$ for linear fitting is 0.165 and the one for second-order fitting is 0.154. These values are approximately consistent with the inverse correlation length $\xi^{-1} \cong 0.175$ by means of the density matrix renormalization group method [15].

The estimate $g_{\mathrm{c}}(\infty)$ is almost zero in the region $0 \leq \alpha \lesssim 0.25$ and is finite in the region $0.25 \lesssim \alpha \leq 0.5$. This is consistent with the massive-massless transition [23] at $\alpha \cong 0.2411$ if we admit that $g_{\mathrm{c}}(\infty)$ is equal to the inverse correlation length. (We here comment that the jump of the estimate $g_{\mathrm{c}}(\infty)$ around $\alpha = 0.25$ is caused from inaccuracies of the extrapolation; the energy gap between the first excited state A and the second excited state B at $g = 0$ in Fig. 6.4 (a) becomes almost zero around $\alpha = 0.25$.) It is remarkable that $g_{\mathrm{c}}(\infty)$ is at least approximately equal to the inverse correlation length all through the region $0 \leq \alpha \leq 0.5$ though we do not know the exact dispersion relation of the elementary excitation of this model.

Chapter 7

Summary and discussions

To summarize, we first conjectured that the imaginary part of a zero of the dispersion relation of the elementary excitation in the complex momentum space is equal to the inverse or twice the inverse correlation length. The factor one or two comes from the number of the elementary excitation involved in the excited state. We obtain the dispersion relation in the complex momentum space by analytic continuation of the one on the real axis. We confirmed the equality for several strongly correlated quantum systems, that is, the $S = 1/2$ XY chain in a magnetic field, the Hubbard model in the half-filled case and the $S = 1/2$ antiferromagnetic XXZ chain in the Ising-like region. We also confirmed the equality for unsolved systems, namely, the Majumdar-Ghosh model, whose variational dispersion relations are only obtained. We expect that it may be a universal relation for any strongly correlated quantum systems that the imaginary part of a zero of the dispersion relation of the elementary excitation in the complex momentum space is equal to the inverse correlation length.

We next proposed the method of obtaining the dispersion relation on the axis $\mathrm{Im}\, p = g$ (g is a real positive constant) for the purpose of searching zeros of the dispersion relation in the complex momentum space. The method is to consider a non-Hermitian generalization of strongly correlated quantum systems where an imaginary vector potential is added to the momentum operator; specifically, we multiply the right hopping energy by e^{g} and the left hopping energy by e^{-g}. We argued that we may be able to obtain zeros only by observing the spectral behavior, that is, by looking for the point where the energy gap from the ground state vanishes. We partly analytically confirmed the relation that the non-Hermitian critical point g_{c} where the energy gap vanishes for a non-Hermitian system is equal to the inverse correlation length of a Hermitian system. The relation is valid for the $S = 1/2$ **isotropic** XY chain in a magnetic field; and is suggested to be valid for the Hubbard model in the half-filled case and for the $S = 1/2$ XXZ chain in the Ising-like region. The equality between the non-Hermitian critical point g_{c} of a non-Hermitian system and the inverse correlation length of a Hermitian system is thus equivalent to our conjecture that the imaginary part of a zero of the dispersion relation is equal to the inverse correlation length. We also numerically analyzed the $S = 1/2$ antiferromagnetic Heisenberg chain with the nearest- and the next-nearest-neighbor interactions, which is unsolved analytically. We presented numerical evidence that the extrapolated estimates of the non-Hermitian "critical" point for finite systems is consistent with the inverse correlation length.

We have to admit that our non-Hermitian generalization is not always appropriate for having the inverse correlation length. One example is the NNN Heisenberg chain (6.5) with $\alpha > 0.5$ in the incommensurate state, whose energy gap between the ground state and the excited state have different wave numbers. Another example is the $S = 1/2$ ferromagnetic transverse Ising chain whose elementary excitation is obtained by the Bogoliubov transformation; the creation and annihilation operators at two different wave numbers k and $-k$ are mixed. Other principles of non-Hermitian generalizations for such cases may be needed.

Appendix A

Non-Hermitian analysis of the random Anderson model

We review an application of the non-Hermitian generalization (1.9), which was first discussed by Hatano and Nelson [2] for the random Anderson model. We can estimate the localization length only by observing the energy-spectral flow upon increasing the non-Hermiticity g without calculating the wave function directly. A one-electron non-Hermitian Anderson model in one dimension is given by

$$\mathcal{H} = -t \sum_{x=-\infty}^{\infty} \left(e^{g} |x+1\rangle\langle x| + e^{-g} |x\rangle\langle x+1| \right) + \sum_{x=-\infty}^{\infty} V_x |x\rangle\langle x|, \tag{A.1}$$

where V_x is a random potential at site x. In solving the non-Hermitian Schrödinger equations

$$\begin{aligned} \mathcal{H}\Psi_g^R(x) &= \varepsilon_g \Psi_g^R(x), \\ \Psi_g^L(x)\mathcal{H} &= \varepsilon_g \Psi_g^L(x), \end{aligned} \tag{A.2}$$

we look for the right eigenfunction $\Psi_g^R(x)$ and the left eigenfunction $\Psi_g^L(x)$ in the normalizable functional space. A localized eigenfunction for $g = 0$ is, except for an oscillatory factor, asymptotically given by

$$\Psi_0(x) \sim e^{-\kappa|x|}, \tag{A.3}$$

where κ is the inverse localization length and we set the localization center to $x = 0$ for simplicity. We here introduce the imaginary vector potential $i\hbar g$. We readily see that the right and the left wavefunctions [2]

$$\Psi_g^R(x) = e^{gx}\Psi_0(x), \tag{A.4}$$

$$\Psi_g^L(x) = e^{-gx}\Psi_0(x), \tag{A.5}$$

satisfy Eq. (A.2) with the same eigenvalue as in the Hermitian case, namely $\varepsilon_g = \varepsilon_0$. We refer to Eqs. (A.4) and (A.5) as the imaginary gauge transformation. Equations (A.4) and (A.5) with Eq. (A.3) yield

$$\Psi_g^R(x) \sim e^{gx-\kappa|x|}, \qquad \Psi_g^L(x) \sim e^{-gx-\kappa|x|}, \tag{A.6}$$

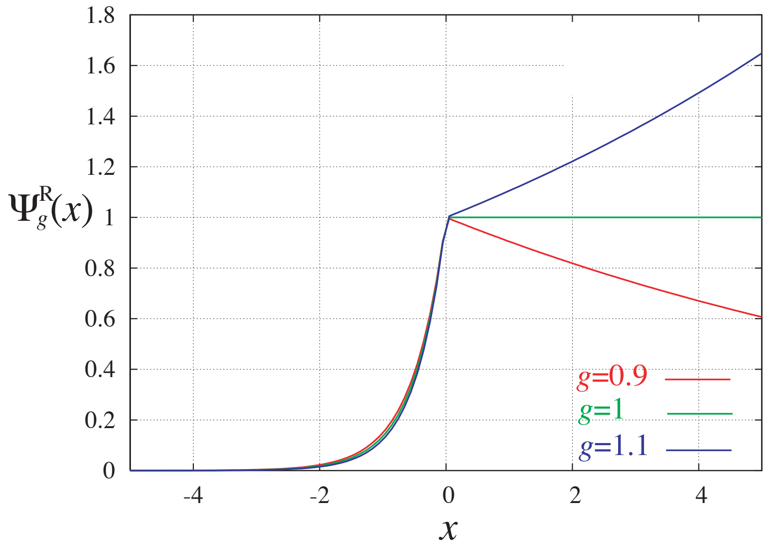


Figure A.1: The right eigenfunction $\Psi_g^R = e^{gx-|x|}$ for $g = 0.9, 1$ and 1.1. The non-Hermitian critical point is $g_c = 1$ in this case.

which is schematically shown in Fig. A.1 for $\kappa = 1$. The right and left eigenfunctions are indeed normalizable for $|g| < \kappa$, that is,

$$\Psi_g^R(\pm\infty) \to 0, \qquad \Psi_g^L(\pm\infty) \to 0, \tag{A.7}$$

and hence they can be solutions of Eq. (A.2) in the normalizable functional space.

However, the solution changes dramatically for $|g| > \kappa$. The functions of the forms (A.4) and (A.5) diverge as

$$\Psi_g^R(+\infty) \to \infty, \qquad \Psi_g^L(-\infty) \to \infty, \tag{A.8}$$

and are not normalizable any more. They are no longer the solution in the normalizable functional space. In fact, an extended wavefunction

$$\Psi_g^{R(L)}(x) \sim e^{ikx} \tag{A.9}$$

with an approximate eigenvalue

$$\varepsilon_g \cong \frac{(\hbar k + i\hbar g)^2}{2m}. \tag{A.10}$$

is permitted [2]. Note that ε_g is a complex number depending on g. In numerical calculations, we can reproduce the above for finite systems under the periodic boundary condition:

$$\mathcal{H} = -t\sum_{x=1}^{L}\left(e^g|x+1\rangle\langle x| + e^{-g}|x\rangle\langle x+1|\right) + \sum_{x=1}^{L} V_x|x\rangle\langle x|, \tag{A.11}$$

where the site $L+1$ is identified with the site 1. The spectrum of periodic systems converge to Eq. (A.10) as $L \to \infty$. The functions (A.4) and (A.5) satisfy the periodic boundary condition for $|g| < \kappa$ because of Eq. (A.7) in the large L limit, while they never satisfy the periodic boundary condition for $|g| > \kappa$ because of Eq. (A.8) in the large L limit. We define the non-Hermitian critical point $g_{\mathrm{c}}(L)$ at which the eigenvalues change from real to complex for system size L. We presume that $g_{\mathrm{c}}(L)$ converges to the inverse localization length κ for the infinite system as $L \to \infty$. We thus estimate the inverse localization length κ only by observing the spectral change, not by calculating the wave function directly. It is a merit of the non-Hermitian generalization.

Appendix B

Non-Hermitian analysis of the $S = 1/2$ transverse Ising chain

We derive an appropriate non-Hermitian version of the $S = 1/2$ ferromagnetic transverse Ising chain

$$\mathcal{H} = -J \sum_{l=1}^{L} S_l^x S_{l+1}^x - h \sum_{l=1}^{L} S_l^z \tag{B.1}$$

by making the momentum k of the elementary excitation transformed to $k + ig$. We argue that the non-Hermitian generalization in Eq. (1.9) is not efficient for this model.

The Hamiltonian (B.1) is transformed into (2.22) by the Jordan-Wigner transformation in Eq. (2.3). By the Fourier transformation (2.23), the Hamiltonian (2.22) is rewritten in the form (2.24). The Hamiltonian (2.24) is then diagonalized in the momentum space in the form (2.27). The elementary excitation in Eq. (2.27) is given by the Bogoliubov transformation (2.25). The dispersion relation $\epsilon(p)$ is given by (2.28).

By replacing p with $p + \mathrm{i}g$ in the dispersion relation $\epsilon(p)$, let us consider the non-Hermitian Hamiltonian of the form

$$\mathcal{H}(g) = \sum_{-\pi<p<\pi} \epsilon(p + \mathrm{i}g) \left(\eta_p^\dagger \eta_p - \frac{1}{2} \right). \tag{B.2}$$

The inverse Bogoliubov transformation of (B.2), after some algebra, gives

$$\begin{aligned}\mathcal{H}(g) =& \frac{1}{2}\sum_{0<p<\pi}\left[\epsilon(p+\mathrm{i}g)-\epsilon(p-\mathrm{i}g)-(J\cos p/2-h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{\epsilon(p)}\right]c_p^\dagger c_p \\ &+\frac{1}{2}\sum_{0<p<\pi}\left[-\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)-(J\cos p/2-h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{\epsilon(p)}\right]c_{-p}^\dagger c_{-p} \\ &-\frac{1}{2}\sum_{0<p<\pi}\frac{J\sin p}{2}\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{\epsilon(p)}(c_p^\dagger c_{-p}^\dagger+c_{-p}c_p) \\ &+\sum_{0<p<\pi}(J\cos p/2-h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)} \\ =& -\sum_{0<p<\pi}\Gamma_1(p)(c_p^\dagger c_p+c_{-p}^\dagger c_{-p})+\sum_{0<p<\pi}\Gamma_2(p)(c_p^\dagger c_p-c_{-p}^\dagger c_{-p}) \\ &-\sum_{0<p<\pi}\Gamma_3(p)(c_p^\dagger c_{-p}^\dagger+c_{-p}c_p)+\sum_{0<p<\pi}\Gamma_4(p),\end{aligned} \tag{B.3}$$

where

$$\begin{aligned}\Gamma_1(p) &= (J\cos p/2-h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}, \\ \Gamma_2(p) &= \frac{\epsilon(p+\mathrm{i}g)-\epsilon(p-\mathrm{i}g)}{2}, \\ \Gamma_3(p) &= \frac{J\sin p}{2}\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}, \\ \Gamma_4(p) &= (J\cos p/2-h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}.\end{aligned} \tag{B.4}$$

We rewrite $\Gamma_1(p), \Gamma_2(p)$ and $\Gamma_3(p)$ by the Fourier-series expansions

$$\Gamma_1(p) = 2\sum_{n=0}^{\infty}\alpha_n\cos(np), \quad \Gamma_2(p) = -2\mathrm{i}\sum_{n=0}^{\infty}\beta_n\sin(np), \quad \Gamma_3(p) = -2\sum_{n=0}^{\infty}\gamma_n\sin(np), \tag{B.5}$$

where the coefficients α_n, β_n and γ_n are given by the following integrals:

$$\begin{aligned}\alpha_n &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\Gamma_1(p)\cos(np)dp = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{J\cos p}{2}-h\right)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}\cos(np)\mathrm{d}p, \\ \beta_n &= \frac{\mathrm{i}}{2\pi}\int_{-\pi}^{\pi}\Gamma_2(p)\sin(np)dp = \frac{\mathrm{i}}{2\pi}\int_{-\pi}^{\pi}\frac{\epsilon(p+\mathrm{i}g)-\epsilon(p-\mathrm{i}g)}{2}\sin(np)\mathrm{d}p, \\ \gamma_n &= -\frac{1}{2\pi}\int_{-\pi}^{\pi}\Gamma_3(p)\sin(np)dp = -\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{J\sin p}{2}\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}\sin(np)\mathrm{d}p.\end{aligned} \tag{B.6}$$

We thus the Hamiltonian (B.2) rewritten in the form

$$\mathcal{H}(g) = \sum_l\sum_{n=1}^{\infty}\left[(-\alpha_n+\beta_n)c_{l+n}^\dagger c_l+(-\alpha_n-\beta_n)c_l^\dagger c_{l+n}-\gamma_n(c_{l+n}^\dagger c_l^\dagger+c_lc_{l+n})\right]-2\alpha_0\sum_l c_l^\dagger c_l+C \tag{B.7}$$

in the real space. By the inverse Jordan-Wigner transformation, we further have

$$
\begin{aligned}
&\mathcal{H}(g)\\
&=\sum_l \sum_{n=1}^{\infty} (-2)^{n-1} S^z_{l+1} \dots S^z_{l+n-1} \left[(-\alpha_n+\beta_n) S^+_{l+n} S^-_l + (-\alpha_n-\beta_n) S^+_l S^-_{l+n} + \gamma_n (S^+_{l+n} S^+_l + S^-_l S^-_{l+n})\right]\\
&\quad - 2\alpha_0 \sum_l S^z_l - \alpha_0 L + C\\
&=\sum_l \sum_{n=1}^{\infty} (-2)^{n} S^z_{l+1} \dots S^z_{l+n-1} \left[(\alpha_n-\gamma_n) S^x_{l+n} S^x_l + (\alpha_n+\gamma_n) S^y_{l+n} S^y_l + \mathrm{i}\beta_n (S^x_{l+n} S^y_l - S^y_{l+n} S^x_l)\right]\\
&\quad - 2\alpha_0 \sum_l S^z_l,
\end{aligned}
\tag{B.8}
$$

where

$$
C \equiv \frac{L}{2\pi}\int_0^{\pi} \Gamma_4(p)dp = \frac{L}{2\pi}\int_0^{\pi} \Gamma_1(p)dp = \frac{L}{2\pi}\int_0^{\pi} (J\cos p/2 - h)\frac{\epsilon(p+\mathrm{i}g)+\epsilon(p-\mathrm{i}g)}{2\epsilon(p)}dp. \tag{B.9}
$$

We note that

$$
-\alpha_0 L + C = -\frac{L}{4\pi}\int_{-\pi}^{\pi} \Gamma_1(p)dp + \frac{L}{2\pi}\int_0^{\pi} \Gamma_1(p)dp = 0. \tag{B.10}
$$

We can see from Eq. (B.8) that the non-Hermitian Hamiltonian is very complicated; interactions between spins beyond the nearest neighbor sites emerge as soon as g is finite. It is because its elementary excitation is obtained by the Bogoliubov transformation; the creation and annihilation operators at two different wave numbers p and $-p$ are mixed. Conversely, the non-Hermitian generalization of the simple form (1.9) does not produce the dispersion relation $\epsilon(p+\mathrm{i}g)$ in this model. We may need another principle of non-Hermitian generalization for this case.

Appendix C

Equality of $g_\mathbf{c}$ and $1/\xi$ for the Hubbard model

We show for the Hubbard model that the non-Hermitian critical point g_c in Eq. (3.12) for the non-Hermitian model and the inverse correlation length $1/\xi$ in Eq. (3.2) for the Hermitian model are actually equal. The non-Hermitian critical point g_c is given by

$$\begin{aligned} g_\mathrm{c} &= \lim_{\Lambda\to\infty}\left[\mathrm{arcsinh}(U/4t) + 2\mathrm{i}\int_{-\Lambda}^{\Lambda}\arctan\frac{\lambda+\mathrm{i}U/4t}{U/4t}\sigma(\lambda)\mathrm{d}\lambda\right] \\ &= \lim_{\Lambda\to\infty}\left[\mathrm{arcsinh}(U/4t) + \frac{\mathrm{i}}{\pi}\int_{-\Lambda}^{\Lambda}\mathrm{d}\lambda\arctan\frac{\lambda+\mathrm{i}U/4t}{U/4t}\int_0^\infty\frac{\cos(\omega\lambda)J_0(\omega)}{\cosh((U/4t)\omega)}\mathrm{d}\omega\right], \end{aligned} \tag{C.1}$$

where $\sigma(\lambda)$ is a distribution function of the spin rapidity λ given in Eq. (3.32). Using the variable transformation

$$\theta = \arctan(\lambda/(U/4t) + \mathrm{i}) \tag{C.2}$$

with

$$\tan\theta_1 = -\frac{\Lambda}{U/4t} + \mathrm{i}, \quad \tan\theta_2 = \frac{\Lambda}{U/4t} + \mathrm{i}, \tag{C.3}$$

we have

$$\begin{aligned} g_\mathrm{c} &= \lim_{\Lambda\to\infty}\left[\mathrm{arcsinh}(U/4t) + \frac{\mathrm{i}}{\pi}\int_{\theta_1}^{\theta_2}\frac{(U/4t)\theta}{\cos^2\theta}\int_0^\infty\frac{\cos((U/4t)\omega\tan\theta - \mathrm{i}(U/4t)\omega)J_0(\omega)\mathrm{d}\omega}{\cosh((U/4t)\omega)}\mathrm{d}\theta\right] \\ &= \lim_{\Lambda\to\infty}\left[\mathrm{arcsinh}(U/4t) + \frac{\mathrm{i}}{\pi}\int_0^\infty\frac{(U/4t)J_0(\omega)\mathrm{d}\omega}{\cosh((U/4t)\omega)}\right. \\ &\quad\left.\times\left\{\underbrace{\left[\frac{\sin((U/4t)\omega\tan\theta - \mathrm{i}(U/4t)\omega)}{(U/4t)\omega}\theta\right]_{\theta_1}^{\theta_2}}_{I_1} - \underbrace{\int_{\theta_1}^{\theta_2}\frac{\sin((U/4t)\omega\tan\theta - \mathrm{i}(U/4t)\omega)}{(U/4t)\omega}\mathrm{d}\theta}_{I_2}\right\}\right]. \end{aligned} \tag{C.4}$$

We rewrite the term I_1 in the form

$$\begin{aligned}I_1 =&\frac{1}{(U/4t)\omega}\left[\theta_2\sin((U/4t)\omega\tan\theta_2 - \mathrm{i}(U/4t)\omega) - \theta_1\sin((U/4t)\omega\tan\theta_1 - \mathrm{i}(U/4t)\omega)\right]\\ =&\frac{1}{(U/4t)\omega}(\theta_1+\theta_2)\sin(\omega\Lambda), \qquad \text{(C.5)}\end{aligned}$$

where the coefficients θ_1 and θ_2 for $\Lambda \gg 1$ take the form

$$\theta_1 = -\frac{\pi}{2} - \delta_1, \quad \theta_2 = \frac{\pi}{2} - \delta_2 \qquad \text{(C.6)}$$

with $|\delta_1|, |\delta_2| \ll 1$. Because of

$$\tan\theta_1 = \frac{1}{\tan\delta_1} \simeq \frac{1}{\delta_1}, \qquad \tan\theta_2 = \frac{1}{\tan\delta_2} \simeq \frac{1}{\delta_2}, \qquad \text{(C.7)}$$

we have

$$\begin{aligned}I_1 &= \frac{1}{(U/4t)\omega}(-\delta_1-\delta_2)\sin(\omega\Lambda)\\ &= \frac{1}{(U/4t)\omega}\left(-\frac{U/4t}{\mathrm{i}(U/4t)-\Lambda} - \frac{U/4t}{\mathrm{i}(U/4t)+\Lambda}\right)\sin(\omega\Lambda)\\ &= \frac{2\mathrm{i}(U/4t)}{\omega((U/4t)^2+\Lambda^2)}\sin(\omega\Lambda)\\ &\xrightarrow{\Lambda\to\infty} 0. \qquad \text{(C.8)}\end{aligned}$$

Next we calculate the integral I_2 in Eq. (C.4). By using the variable transformation $x = \tan\theta - \mathrm{i}$, we have

$$\begin{aligned}I_2 &= \lim_{\Lambda\to\infty}\int_{-\Lambda/(U/4t)}^{\Lambda/(U/4t)} \frac{\sin((U/4t)\omega x)}{(U/4t)\omega}\frac{\mathrm{d}x}{1+(x+\mathrm{i})^2}\\ &= \int_{-\infty}^{\infty}\frac{\sin((U/4t)\omega x)}{(U/4t)\omega(x^2+2\mathrm{i}x)}\mathrm{d}x = \frac{\pi}{2\mathrm{i}(U/4t)\omega}(1-e^{-2|\omega|(U/4t)}). \qquad \text{(C.9)}\end{aligned}$$

We thus arrive at

$$\begin{aligned}g_{\mathrm{c}} =&\operatorname{arcsinh}(U/4t) - \frac{\mathrm{i}}{\pi}\int_0^\infty \frac{(U/4t)J_0(\omega)}{\cosh((U/4t)\omega)}\frac{\pi}{2\mathrm{i}(U/4t)\omega}(1-e^{-2|\omega|(U/4t)})\mathrm{d}\omega\\ =&\operatorname{arcsinh}(U/4t) - 2\int_0^\infty \frac{J_0(\omega)\sinh((U/4t)\omega)}{\omega(1+e^{\omega U/2t})}\mathrm{d}\omega. \qquad \text{(C.10)}\end{aligned}$$

We thus confirmed that the expression (C.10), or Eq. (3.12) is actually equal to the inverse correlation length of the charge excitation (3.2).

Appendix D

Lieb-Wu equation for the non-Hermitian Hubbard model

We derive Lieb-Wu equation for the non-Hermitian Hubbard model [3]:

$$\mathcal{H} = -t \sum_{l=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{g} c_{l+1,\sigma}^{\dagger} c_{l,\sigma} + e^{-g} c_{l,\sigma}^{\dagger} c_{l+1,\sigma}) + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}. \tag{D.1}$$

We prepare the right eigenfunction $|N, M\rangle$ with N electrons and with M down spins;

$$|N, M\rangle = \sum_{\{\sigma_j\}} \sum_{\{x_j\}} \Psi_g^{(R)}(x_1, x_2, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N) c_{x_1,\sigma_1}^{\dagger} \cdots c_{x_N,\sigma_N}^{\dagger} |0\rangle. \tag{D.2}$$

Considering the Fermion's anticommutation relation, we impose the condition

$$\Psi_g^{(R)}(x_{P_1}, x_{P_2}, \cdots, x_{P_N}; \sigma_{P_1}, \sigma_{P_2}, \cdots, \sigma_{P_N}) = \mathrm{sgn}(P) \Psi_g^{(R)}(x_1, x_2, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N), \tag{D.3}$$

where $P = (P_1, P_2, \cdots, P_N)$ is a permutation of the labels $1, 2, \cdots, N$. The Schrödinger equation for the right eigenfunction $\Psi_g^{(R)}$ is

$$\begin{aligned}
&- te^{-g} \sum_{j=1}^{N} \Psi_g^{(R)}(x_1, \cdots, x_j + 1, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N) \\
&- te^{g} \sum_{j=1}^{N} \Psi_g^{(R)}(x_1, \cdots, x_j - 1, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N) \\
&+ U \sum_{x_j < x_k} \delta(x_j, x_k) \Psi_g^{(R)}(x_1, \cdots, x_j, \cdots, x_k, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N) \\
&= E \Psi_g^{(R)}(x_1, \cdots, x_j, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N),
\end{aligned} \tag{D.4}$$

where E is an eigenenergy. In order to diagonalize the Hamiltonian (D.1), we make the ansatz for the right eigenfunction $\Psi_g^{(R)}$ of the form

$$\begin{aligned}
&\Psi_g^{(R)}(x_1, x_2, \cdots, x_N; \sigma_1, \sigma_2, \cdots, \sigma_N) \\
&= \sum_{\{P\}} \mathrm{sgn}(PQ) A_{\sigma_{Q_1}, \cdots, \sigma_{Q_N}}(k_{P_1}, \cdots, k_{P_N}) \exp\left(\mathrm{i} \sum_{j=1}^{N} (k_{P_j} - \mathrm{i}g) x_{Q_j} \right)
\end{aligned} \tag{D.5}$$

under the condition

$$1 \leq x_{Q_1} \leq x_{Q_2} \leq \cdots \leq x_{Q_N} \leq L. \tag{D.6}$$

In the case $x_{Q_1} < x_{Q_2} < \cdots < x_{Q_N}$, the Schrödinger equation (D.4) is reduced to

$$\sum_{\{P\}} \mathrm{sgn}(PQ) A_{\sigma_{Q_1},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_N}) \sum_{j=1}^{N} (-te^{\mathrm{i}k_{P_j}} - te^{-\mathrm{i}k_{P_j}}) \exp\left(\mathrm{i}\sum_{j=1}^{N}(k_{P_j} - \mathrm{i}g)x_{Q_j}\right)$$
$$= E\sum_{\{P\}} \mathrm{sgn}(PQ) A_{\sigma_{Q_1},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_N}) \exp\left(\mathrm{i}\sum_{j=1}^{N}(k_{P_j} - \mathrm{i}g)x_{Q_j}\right). \tag{D.7}$$

We therefore obtain the eigenenergy E of the form

$$E = -2t\sum_{j=1}^{N}\cos k_{P_j} = -2t\sum_{j=1}^{N}\cos k_j. \tag{D.8}$$

We next consider the case $x_{Q_i} = x_{Q_{i+1}} = x$, where $Q_i = a$ and $Q_{i+1} = b$ are assumed. We derive two sets of equations. First, the continuity of the wavefunction $\Psi_g^{(R)}$ at $x_a = x_b = x$ requires

$$\begin{aligned} &A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}) \\ &- A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N}) \\ =&- A_{\sigma_{Q_1},\cdots,\sigma_{Q_{i+1}},\sigma_{Q_i},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}) \\ &+ A_{\sigma_{Q_1},\cdots,\sigma_{Q_{i+1}},\sigma_{Q_i},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N}). \end{aligned} \tag{D.9}$$

Next, we use $\Psi_g^{(R)}(x_1,\cdots,x_a,\cdots,x_b,\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N)$
$= \Psi_g^{(R)}(x_1,\cdots,x,\cdots,x,\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N)$ in the Schrödinger equation (D.4). By taking all terms proportional to $e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)x_{Q_1}+\cdots+\mathrm{i}(k_{P_i}-\mathrm{i}g)x+\mathrm{i}(k_{P_{i+1}}-\mathrm{i}g)x+\cdots+\mathrm{i}(k_{P_N}-\mathrm{i}g)x_{Q_N}}$, we obtain the relation

$$\begin{aligned} &A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}) \\ &\quad\times[te^{\mathrm{i}k_{P_{i+1}}} + te^{-\mathrm{i}k_{P_i}} - 2t\cos k_{P_i} - 2t\cos k_{P_{i+1}} - U] \\ &-A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N}) \\ &\quad\times[te^{\mathrm{i}k_{P_i}} + te^{-\mathrm{i}k_{P_{i+1}}} - 2t\cos k_{P_i} - 2t\cos k_{P_{i+1}} - U] \\ &-A_{\sigma_{Q_1},\cdots,\sigma_{Q_{i+1}},\sigma_{Q_i},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N})[te^{\mathrm{i}k_{P_{i+1}}} + te^{-\mathrm{i}k_{P_i}}] \\ &+A_{\sigma_{Q_1},\cdots,\sigma_{Q_{i+1}},\sigma_{Q_i},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N})[te^{\mathrm{i}k_{P_i}} + te^{-\mathrm{i}k_{P_{i+1}}}] \\ &\quad= 0. \end{aligned} \tag{D.10}$$

By using the sets of equations (D.9) and (D.10), we have

$$\begin{aligned} &A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N}) \\ =&\frac{-U/2\mathrm{i}t}{\sin k_{P_i} - \sin k_{P_{i+1}} - U/2\mathrm{i}t} A_{\sigma_{Q_1},\cdots,\sigma_{Q_i},\sigma_{Q_{i+1}},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}) \\ +&\frac{\sin k_{P_i} - \sin k_{P_{i+1}}}{\sin k_{P_i} - \sin k_{P_{i+1}} - U/2\mathrm{i}t} A_{\sigma_{Q_1},\cdots,\sigma_{Q_{i+1}},\sigma_{Q_i},\cdots,\sigma_{Q_N}}(k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}). \end{aligned} \tag{D.11}$$

We now define a particular set of state in the spin chain:

$$|k_{P_1},\cdots,k_{P_N}\rangle = \sum_{\{\sigma_i\}=\uparrow,\downarrow} A_{\sigma_1,\sigma_2,\cdots,\sigma_N}(k_{P_1},k_{P_2},\cdots,k_{P_N})|\sigma_1,\sigma_2,\cdots,\sigma_N\rangle. \tag{D.12}$$

We thus map the problem in the space of $(N!)^2$ dimensions to a problem in the space of 2^N dimensions. We then introduce an operator $Y^{(a,b)}(x)$ of the form

$$Y^{(a,b)}(x) \equiv \underbrace{\frac{-U/2\mathrm{i}t}{x-U/2\mathrm{i}t}}_{\equiv\alpha(x)} I + \underbrace{\frac{x}{x-U/2\mathrm{i}t}}_{\equiv\beta(x)} \Pi^{(a,b)}, \tag{D.13}$$

where the operator $\Pi^{(a,b)}$ is an exchange operator defined by

$$|\sigma_1,\cdots,\sigma_b,\cdots,\sigma_a,\cdots,\sigma_N\rangle = \Pi^{(a,b)}|\sigma_1,\cdots,\sigma_a,\cdots,\sigma_b,\cdots,\sigma_N\rangle. \tag{D.14}$$

We can easily show that

$$Y^{(a,b)}(\sin k_{P_i}-\sin k_{P_{i+1}})|k_{P_1},\cdots,k_{P_i},k_{P_{i+1}},\cdots,k_{P_N}\rangle = |k_{P_1},\cdots,k_{P_{i+1}},k_{P_i},\cdots,k_{P_N}\rangle \tag{D.15}$$

by considering Eqs. (D.11) and (D.13).

We next map the periodic boundary conditions

$$\begin{aligned}&\Psi_g^{(R)}(x_1,\cdots,x_{j-1},0,x_{j+1},\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N)\\=&\Psi_g^{(R)}(x_1,\cdots,x_{j-1},L,x_{j+1},\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N)\end{aligned} \tag{D.16}$$

and

$$\begin{aligned}&\Psi_g^{(R)}(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N)\\=&\Psi_g^{(R)}(x_1,\cdots,x_{j-1},L+1,x_{j+1},\cdots,x_N;\sigma_1,\sigma_2,\cdots,\sigma_N),\end{aligned} \tag{D.17}$$

where $Q_1 = j$ is assumed, in the space of $(N!)^2$ dimensions to the space of 2^N dimensions. By inserting Eq. (D.5) into Eq. (D.17), we obtain

$$A_{\sigma_{Q_1},\sigma_{Q_2}\cdots,\sigma_{Q_N}}(k_{P_1},k_{P_2},\cdots,k_{P_N}) = e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} A_{\sigma_{Q_2}\cdots,\sigma_{Q_N},\sigma_{Q_1}}(k_{P_2},\cdots,k_{P_N},k_{P_1}). \tag{D.18}$$

We thus have

$$
\begin{aligned}
|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle &= \sum_{\{\sigma_i\}=\uparrow,\downarrow} A_{\sigma_1,\sigma_2\cdots,\sigma_N}(k_{P_1}, \cdots, k_{P_N})|\sigma_1, \sigma_2, \cdots, \sigma_N\rangle \\
=& e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \sum_{\{\sigma_i\}=\uparrow,\downarrow} A_{\sigma_2,\cdots,\sigma_N,\sigma_1}(k_{P_2}, \cdots, k_{P_N}, k_{P_1}) \prod_{j=1}^{N-1} \Pi^{(j,j+1)}|\sigma_2, \cdots, \sigma_N, \sigma_1\rangle \\
=& e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \prod_{j=1}^{N-1} \Pi^{(j,j+1)} \sum_{\{\sigma_i\}=\uparrow,\downarrow} A_{\sigma_2,\cdots,\sigma_N,\sigma_1}(k_{P_2}, \cdots, k_{P_N}, k_{P_1})|\sigma_2, \cdots, \sigma_N, \sigma_1\rangle \\
=& e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \prod_{j=1}^{N-1} \Pi^{(j,j+1)} \sum_{\{\sigma_i\}=\uparrow,\downarrow} A_{\sigma_1,\cdots,\sigma_N}(k_{P_2}, \cdots, k_{P_N}, k_{P_1})|\sigma_1, \cdots, \sigma_N\rangle \\
=& e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \prod_{j=1}^{N-1} \Pi^{(j,j+1)}|k_{P_2}, \cdots, k_{P_N}, k_{P_1}\rangle \\
=& e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \prod_{l=1}^{N-1} \Pi^{(l,l+1)} \prod_{j=0}^{N-2} Y^{(N-j-1,N-j)}(\sin k_{P_1} - \sin k_{P_{N-j}})|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle \\
=& e^{i(k_{P_1}-ig)L} \prod_{j=0}^{N-2} X^{(1,N-j)}(\sin k_{P_1} - \sin k_{P_{N-j}})|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle, \qquad \text{(D.19)}
\end{aligned}
$$

where we define the operator $X^{(j,k)}(x)$ of the form

$$
X^{(j,k)}(x) \equiv \Pi^{(j,k)} Y^{(j,k)}(x). \qquad \text{(D.20)}
$$

We here introduce an additional site a and define an operator S of the form

$$
S \equiv \prod_{j=0}^{N-1} X^{(a,N-j)}(\sin k_{P_1} - \sin k_{P_{N-j}}). \qquad \text{(D.21)}
$$

We can easily show that

$$
\mathrm{Tr}_{(a)} S \equiv \langle \uparrow_a |S| \uparrow_a\rangle + \langle \downarrow_a |S| \downarrow_a\rangle = \prod_{j=0}^{N-2} X^{(1,N-j)}(\sin k_{P_1} - \sin k_{P_{N-j}}) \qquad \text{(D.22)}
$$

From Eqs. (D.19) and (D.22), we have

$$
|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle = e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L} \mathrm{Tr}_{(a)} S |k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle. \qquad \text{(D.23)}
$$

In order to calculate $\mathrm{Tr}_{(a)} S$, we introduce the Yang-Baxter relation for the X operator:

$$
X^{(j,k)}(\lambda - \mu) X^{(j,l)}(\lambda) X^{(k,l)}(\mu) = X^{(k,l)}(\mu) X^{(j,l)}(\lambda) X^{(j,k)}(\lambda - \mu), \qquad \text{(D.24)}
$$

which is proved after some elementary algebra. By operating $\Pi^{(k,l)}$ to both hand sides in Eq. (D.24), we obtain the relation

$$
X^{(j,l)}(\lambda - \mu) X^{(j,k)}(\lambda) Y^{(k,l)}(\mu) = Y^{(k,l)}(\mu) X^{(j,l)}(\lambda) X^{(j,k)}(\lambda - \mu). \qquad \text{(D.25)}
$$

We here introduce additional sites a and b. On the basis $|\sigma_a, \sigma_b, \sigma_1, \cdots, \sigma_N\rangle$, the Yang-Baxter equation

$$Y^{(a,b)}(\lambda-\mu)X^{(a,l)}(\lambda)X^{(b,l)}(\mu) = X^{(a,l)}(\mu)X^{(b,l)}(\lambda)Y^{(a,b)}(\lambda-\mu) \tag{D.26}$$

is satisfied for $l = 1, 2, \cdots, N$. By using the Yang-Baxter relation (D.26) recursively, we prove that

$$Y^{(a,b)}(\lambda-\mu)T^{(a)}(\lambda)T^{(b)}(\mu) = T^{(a)}(\mu)T^{(b)}(\lambda)Y^{(a,b)}(\lambda-\mu), \tag{D.27}$$

where we define $T^{(a)}(\lambda)$ of the form

$$T^{(a)}(\lambda) \equiv X^{(a,N)}(\lambda-\lambda_N)\cdots X^{(a,1)}(\lambda-\lambda_1), \tag{D.28}$$

with $\lambda_j \equiv \sin k_{P_j} - U/4\mathrm{i}t$. On the basis $|\uparrow_a\rangle$ and $|\downarrow_a\rangle$, we set elements of $T^{(a)}(\lambda)$ as follows:

$$T^{(a)}(\lambda) \equiv \begin{matrix} & |\uparrow_a\rangle \quad |\downarrow_a\rangle \\ \begin{matrix}\langle\uparrow_a| \\ \langle\downarrow_a|\end{matrix} & \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} \end{matrix}, \tag{D.29}$$

where A, B, C and D are all matrices of 2^{N+1} dimensions. We can show by mathematic induction the following relations:

$$\begin{aligned}
&A(\lambda)|\mathrm{vac}\rangle = |\mathrm{vac}\rangle, \\
&C(\lambda)|\mathrm{vac}\rangle = 0, \\
&D(\lambda)|\mathrm{vac}\rangle = \prod_{j=1}^{N}\left(\frac{\lambda-\lambda_j}{\lambda-\lambda_j-U/2\mathrm{i}t}\right)|\mathrm{vac}\rangle = \prod_{j=1}^{N}\left(\frac{\lambda-\sin k_{P_j}+U/4\mathrm{i}t}{\lambda-\sin k_{P_j}-U/4\mathrm{i}t}\right)|\mathrm{vac}\rangle \equiv d(\lambda)|\mathrm{vac}\rangle,
\end{aligned} \tag{D.30}$$

where we define the vacuum state $|\mathrm{vac}\rangle$ as the state where all spins are up. We can prove Eq. (D.30) by rewriting the operator $X^{(a,j)}(\lambda-\lambda_j)$ in the form

$$X^{(a,j)}(\lambda-\lambda_j) = \begin{pmatrix} \dfrac{(\lambda-\lambda_j-U/4\mathrm{i}t)I-(U/4\mathrm{i}t)\sigma_j^z}{\lambda-\lambda_1-U/2\mathrm{i}t} & \dfrac{-(U/2\mathrm{i}t)\sigma_j^-}{\lambda-\lambda_j-U/2\mathrm{i}t} \\ \dfrac{-(U/2\mathrm{i}t)\sigma_j^+}{\lambda-\lambda_j-U/2\mathrm{i}t} & \dfrac{(\lambda-\lambda_j-U/4\mathrm{i}t)I+(U/4\mathrm{i}t)\sigma_j^z}{\lambda-\lambda_1-U/2\mathrm{i}t} \end{pmatrix}, \tag{D.31}$$

where σ_j^z, σ_j^+ and σ_j^- are 2×2 Pauli matrices acting on site j.

We next derive relations involving A, B, C and D. The operator $Y^{(a,b)}(x)$ is given by

$$Y^{(a,b)}(x) = \begin{matrix} & |\uparrow_a\uparrow_b\rangle \quad |\uparrow_a\downarrow_b\rangle \quad |\downarrow_a\uparrow_b\rangle \quad |\downarrow_a\downarrow_b\rangle \\ \begin{matrix}\langle\uparrow_a\uparrow_b| \\ \langle\uparrow_a\downarrow_b| \\ \langle\downarrow_a\uparrow_b| \\ \langle\downarrow_a\downarrow_b|\end{matrix} & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(x) & c(x) & 0 \\ 0 & c(x) & b(x) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{matrix}, \tag{D.32}$$

where

$$b(x) \equiv \frac{-U/2\mathrm{i}t}{x - U/2\mathrm{i}t}, \quad c(x) \equiv \frac{x}{x - U/2\mathrm{i}t}. \tag{D.33}$$

By substituting Eqs. (D.29) and (D.32) to Eq. (D.27), we obtain sixteen ($= 4 \times 4$) equalities among A, B, C and D. We hereafter use the matrix elements of row 1 and column 4, row 1 and column 3 and row 2 and column 4 to obtain the following equalities:

$$\begin{aligned} &B(\lambda)B(\mu) = B(\mu)B(\lambda), \\ &B(\lambda)A(\mu) = c(\lambda-\mu)A(\mu)B(\lambda) + b(\lambda-\mu)B(\mu)A(\lambda), \\ &b(\lambda-\mu)B(\mu)D(\lambda) + c(\lambda-\mu)D(\lambda)B(\mu) = D(\mu)B(\lambda), \end{aligned} \tag{D.34}$$

or

$$\begin{aligned} B(\lambda)B(\mu) &= B(\mu)B(\lambda), \\ A(\mu)B(\lambda) &= \frac{1}{c(\lambda-\mu)}B(\lambda)A(\mu) - \frac{b(\lambda-\mu)}{c(\lambda-\mu)}B(\mu)A(\lambda), \\ D(\mu)B(\lambda) &= \frac{1}{c(\mu-\lambda)}B(\lambda)D(\mu) - \frac{b(\mu-\lambda)}{c(\mu-\lambda)}B(\mu)D(\lambda). \end{aligned} \tag{D.35}$$

We make the ansatz for the eigenfunction $|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle$ of the form

$$|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle = B(\Lambda_1)B(\Lambda_2)\cdots B(\Lambda_M)|\mathrm{vac}\rangle \tag{D.36}$$

by introducing M parameters $\Lambda_1, \cdots, \Lambda_M$. The eigenvalue equation (D.23) becomes

$$|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle = e^{\mathrm{i}(k_{P_1} - \mathrm{i}g)L}\left[A(\sin k_{P_1} - U/4\mathrm{i}t) + D(\sin k_{P_1} - U/4\mathrm{i}t)\right]|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle. \tag{D.37}$$

We calculate $(A(\lambda) + D(\lambda))|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle$. By using

$$\begin{aligned} A(\lambda)|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle &= \prod_{j=1}^{M} \frac{1}{c(\Lambda_j - \lambda)}|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle \\ &+ \sum_{j=1}^{M} \frac{-b(\Lambda_j - \lambda)}{c(\Lambda_j - \lambda)} \prod_{k=1,k\neq j}^{M} \frac{1}{c(\Lambda_k - \Lambda_j)} B(\lambda)B(\Lambda_1)\cdots B(\Lambda_{j-1})B(\Lambda_{j+1})\cdots B(\Lambda_M)|0 \end{aligned} \tag{D.38}$$

and

$$\begin{aligned} D(\lambda)|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle &= d(\lambda)\prod_{j=1}^{M} \frac{1}{c(\lambda - \Lambda_j)}|k_{P_1}, k_{P_2}, \cdots, k_{P_N}\rangle \\ &+ \sum_{j=1}^{M} \frac{-b(\lambda - \Lambda_j)d(\Lambda_j)}{c(\lambda - \Lambda_j)} \prod_{k=1,k\neq j}^{M} \frac{1}{c(\Lambda_j - \Lambda_k)} B(\lambda)B(\Lambda_1)\cdots B(\Lambda_{j-1})B(\Lambda_{j+1})\cdots B(\Lambda_M)|0\rangle, \end{aligned} \tag{D.39}$$

we have

$$
\begin{aligned}
&(A(\lambda)+D(\lambda))|k_{P_1},k_{P_2},\cdots,k_{P_N}\rangle \\
=&\left(\prod_{j=1}^{M}\frac{1}{c(\Lambda_j-\lambda)}+d(\lambda)\prod_{j=1}^{M}\frac{1}{c(\lambda-\Lambda_j)}\right)|k_{P_1},k_{P_2},\cdots,k_{P_N}\rangle \\
&+\sum_{j=1}^{M}\left(-\frac{b(\Lambda_j-\lambda)}{c(\Lambda_j-\lambda)}\prod_{k=1,k\neq j}^{M}\frac{1}{c(\Lambda_k-\Lambda_j)}-\frac{b(\lambda-\Lambda_j)d(\Lambda_j)}{c(\lambda-\Lambda_j)}\prod_{k=1,k\neq j}^{M}\frac{1}{c(\Lambda_j-\Lambda_k)}\right) \\
&\times B(\lambda)B(\Lambda_1)\cdots B(\Lambda_{j-1})B(\Lambda_{j+1})\cdots B(\Lambda_M)|0\rangle. \qquad \text{(D.40)}
\end{aligned}
$$

The condition that the state $|k_{P_1},k_{P_2},\cdots,k_{P_N}\rangle$ should be an eigenstate of the operator $A(\lambda)+D(\lambda)$ with $\lambda=\sin k_{P_1}-U/4it$ requires

$$
-\frac{b(\Lambda_j-\lambda)}{c(\Lambda_j-\lambda)}\prod_{k=1,k\neq j}^{M}\frac{1}{c(\Lambda_k-\Lambda_j)}-\frac{b(\lambda-\Lambda_j)d(\lambda_j)}{c(\lambda-\Lambda_j)}\prod_{k=1,k\neq j}^{M}\frac{1}{c(\Lambda_j-\Lambda_k)}=0 \qquad \text{(D.41)}
$$

for $j=1,\cdots,M$. From Eq. (D.41), we have

$$
\prod_{l=1}^{N}\left(\frac{\Lambda_j-\sin k_{P_l}+U/4\mathrm{i}t}{\Lambda_j-\sin k_{P_l}-U/4\mathrm{i}t}\right)=-\prod_{k=1}^{M}\left(\frac{\Lambda_j-\Lambda_k+U/2\mathrm{i}t}{\Lambda_j-\Lambda_k-U/2\mathrm{i}t}\right) \qquad (j=1,\cdots,M), \qquad \text{(D.42)}
$$

If the relation (D.42) is satisfied for $j=1,\cdots,M$, the eigenvalue equation (D.37) for the eigenstate $|k_{P_1},k_{P_2},\cdots,k_{P_N}\rangle$ is reduced to

$$
\begin{aligned}
1=&e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L}\left(\prod_{j=1}^{M}\frac{1}{c(\Lambda_j-\sin k_{P_1}+U/4\mathrm{i}t)}+d(\sin k_{P_1}-U/4\mathrm{i}t)\prod_{j=1}^{M}\frac{1}{c(\sin k_{P_1}-\Lambda_j-U/4\mathrm{i}t)}\right) \\
=&e^{\mathrm{i}(k_{P_1}-\mathrm{i}g)L}\prod_{j=1}^{M}\left(\frac{\Lambda_j-\sin k_{P_1}-U/4\mathrm{i}t}{\Lambda_j-\sin k_{P_1}+U/4\mathrm{i}t}\right), \qquad \text{(D.43)}
\end{aligned}
$$

using $d(\sin k_{P_1}-U/4\mathrm{i}t)=0$. We thus obtain the Lieb-Wu equation of the non-Hermitian Hubbard model (D.1) as follows:

$$
\begin{aligned}
\exp(\mathrm{i}Lk_j+gL)&=\prod_{\beta=1}^{M}\frac{\sin k_j-\Lambda_\beta+\mathrm{i}U/4t}{\sin k_j-\Lambda_\beta-\mathrm{i}U/4t} \qquad (j=1,\ldots,N), \\
\prod_{j=1}^{N}\frac{\sin k_j-\Lambda_\alpha+\mathrm{i}U/4t}{\sin k_j-\Lambda_\alpha-\mathrm{i}U/4t}&=-\prod_{\beta=1}^{M}\frac{\Lambda_\alpha-\Lambda_\beta-\mathrm{i}U/2t}{\Lambda_\alpha-\Lambda_\beta+\mathrm{i}U/2t} \qquad (\alpha=1,\ldots,M). \qquad \text{(D.44)}
\end{aligned}
$$

Appendix E

Strong coupling expansion of the non-Hermitian t-t'-U model

E.1 Application of MacDonald's technique to the non-Hermitian t-t'-U model

We consider the strongly coupling expansion of the non-Hermitian t-t'-U model (5.14) and derive the effective Hamiltonian (6.5) by applying MacDonald's technique [26]. The non-Hermitian t-t'-U model is

$$\mathcal{H} = \mathcal{T} + \mathcal{V}, \tag{E.1}$$

where

$$\mathcal{T} = -t \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{g\sigma} c_{i+1,\sigma}^{\dagger} c_{i,\sigma} + e^{-g\sigma} c_{i,\sigma}^{\dagger} c_{i+1,\sigma}) - t' \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{2g\sigma} c_{i+2,\sigma}^{\dagger} c_{i,\sigma} + e^{-2g\sigma} c_{i,\sigma}^{\dagger} c_{i+2,\sigma}), \tag{E.2}$$

$$\mathcal{V} = U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow}. \tag{E.3}$$

The real parameter g denotes the non-Hermiticity and σ corresponds to $+1$ for $\sigma =\uparrow$ and -1 for $\sigma =\downarrow$. We divide the hopping-energy term $\mathcal{T}$ into $\mathcal{T}_m$ which increases the number of doubly occupied sites by m. We then have

$$\mathcal{T} \equiv \mathcal{T}_1 + \mathcal{T}_{-1} + \mathcal{T}_1' + \mathcal{T}_{-1}' + \mathcal{T}_0, \tag{E.4}$$

where the operators $\mathcal{T}_{\pm 1}$, $\mathcal{T}'_{\pm 1}$ and $\mathcal{T}_0$ are given by

$$\mathcal{T}_1 = -t \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{g\sigma} n_{i+1,\bar{\sigma}} c^\dagger_{i+1,\sigma} c_{i,\sigma} h_{i,\bar{\sigma}} + e^{-g\sigma} n_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+1,\sigma} h_{i+1,\bar{\sigma}}), \tag{E.5}$$

$$\mathcal{T}_{-1} = -t \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{g\sigma} h_{i+1,\bar{\sigma}} c^\dagger_{i+1,\sigma} c_{i,\sigma} n_{i,\bar{\sigma}} + e^{-g\sigma} h_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+1,\sigma} n_{i+1,\bar{\sigma}}), \tag{E.6}$$

$$\mathcal{T}'_1 = -t' \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{2g\sigma} n_{i+2,\bar{\sigma}} c^\dagger_{i+2,\sigma} c_{i,\sigma} h_{i,\bar{\sigma}} + e^{-2g\sigma} n_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+2,\sigma} h_{i+2,\bar{\sigma}}), \tag{E.7}$$

$$\mathcal{T}'_{-1} = -t' \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{2g\sigma} h_{i+2,\bar{\sigma}} c^\dagger_{i+2,\sigma} c_{i,\sigma} n_{i,\bar{\sigma}} + e^{-2g\sigma} h_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+2,\sigma} n_{i+2,\bar{\sigma}}), \tag{E.8}$$

$$\begin{aligned}\mathcal{T}_0 = & -t \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} \Big(e^{g\sigma} n_{i+1,\bar{\sigma}} c^\dagger_{i+1,\sigma} c_{i,\sigma} n_{i,\bar{\sigma}} + e^{-g\sigma} n_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+1,\sigma} n_{i+1,\bar{\sigma}} \\ & + e^{g\sigma} h_{i+1,\bar{\sigma}} c^\dagger_{i+1,\sigma} c_{i,\sigma} h_{i,\bar{\sigma}} + e^{-g\sigma} h_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+1,\sigma} h_{i+1,\bar{\sigma}} \Big) \\ & - t' \sum_{i=1}^{L} \sum_{\sigma=\uparrow,\downarrow} \Big(e^{2g\sigma} n_{i+2,\bar{\sigma}} c^\dagger_{i+2,\sigma} c_{i,\sigma} n_{i,\bar{\sigma}} + e^{-2g\sigma} n_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+2,\sigma} n_{i+2,\bar{\sigma}} \\ & + e^{2g\sigma} h_{i+2,\bar{\sigma}} c^\dagger_{i+2,\sigma} c_{i,\sigma} h_{i,\bar{\sigma}} + e^{-2g\sigma} h_{i,\bar{\sigma}} c^\dagger_{i,\sigma} c_{i+2,\sigma} h_{i+2,\bar{\sigma}} \Big)\end{aligned} \tag{E.9}$$

with $h_{i,\sigma}$ as $h_{i,\sigma} \equiv 1 - n_{i,\sigma}$. We can immediately derive the following relations:

$$[\mathcal{V},\ \mathcal{T}_{\pm 1}] = \pm U \mathcal{T}_{\pm 1}, \qquad [\mathcal{V},\ \mathcal{T}'_{\pm 1}] = \pm U \mathcal{T}'_{\pm 1}, \qquad [\mathcal{V},\ \mathcal{T}_0] = 0. \tag{E.10}$$

We here introduce a new Hamiltonian $\mathcal{H}'$ of the form

$$\mathcal{H}' \equiv e^{\mathrm{i}\mathcal{S}} \mathcal{H} e^{-\mathrm{i}\mathcal{S}} = \mathcal{H} + \frac{[\mathrm{i}\mathcal{S}, \mathcal{H}]}{1!} + \frac{[\mathrm{i}\mathcal{S}, [\mathrm{i}\mathcal{S}, \mathcal{H}]]}{2!} + \cdots, \tag{E.11}$$

where $\mathcal{S}$ is an operator. All eigenvalues of $\mathcal{H}$ are equal to the ones of $\mathcal{H}'$.

We hereafter obtain the Hamiltonian $\mathcal{H}'^{(k)}$ recursively in the way

$$\mathcal{H}'^{(k)} = e^{\mathrm{i}\mathcal{S}^{(k-1)}} \mathcal{H}'^{(k-1)} e^{-\mathrm{i}\mathcal{S}^{(k-1)}} \tag{E.12}$$

by choosing $e^{\mathrm{i}\mathcal{S}^{(k-1)}}$ so that hopping terms changes the number of doubly occupied sites may not be generated in the order higher than $(1/U)^{k-2}$ in the Hamiltonian $\mathcal{H}'^{(k)}$. We start from the Hamiltonian $\mathcal{H}'^{(1)} \equiv \mathcal{H}$:

$$\mathcal{H}'^{(1)} \equiv \mathcal{H} = \mathcal{V} + \mathcal{T}_1 + \mathcal{T}_{-1} + \mathcal{T}'_1 + \mathcal{T}'_{-1} + \mathcal{T}_0. \tag{E.13}$$

We can eliminate the terms $\mathcal{T}_{\pm 1}$ and $\mathcal{T}'_{\pm 1}$ which change the number of doubly occupied sites by choosing $\mathrm{i}\mathcal{S}^{(1)}$ as

$$\mathrm{i}\mathcal{S}^{(1)} = U^{-1}(\mathcal{T}_1 - \mathcal{T}_{-1} + \mathcal{T}'_1 - \mathcal{T}'_{-1}). \tag{E.14}$$

The transformations $e^{\mathrm{i}\mathcal{S}^{(1)}}$ and $e^{-\mathrm{i}\mathcal{S}^{(1)}}$ are not unitary operators for any finite g. The transformed Hamiltonian $\mathcal{H}'^{(2)}$ is

$$\begin{aligned}\mathcal{H}'^{(2)} &= e^{\mathrm{i}\mathcal{S}^{(1)}}\mathcal{H}'^{(1)}e^{-\mathrm{i}\mathcal{S}^{(1)}} = e^{\mathrm{i}\mathcal{S}^{(1)}}\mathcal{H}e^{-\mathrm{i}\mathcal{S}^{(1)}} \\ &= \mathcal{V} + \mathcal{T}_0 + \frac{1}{U}\left([\mathcal{T}_1,\mathcal{T}_{-1}] + [\mathcal{T}_1,\mathcal{T}'_{-1}] + [\mathcal{T}'_1,\mathcal{T}_{-1}] + [\mathcal{T}'_1,\mathcal{T}'_{-1}]\right. \\ &\quad \left. +[\mathcal{T}_1,\mathcal{T}_0] + [\mathcal{T}_0,\mathcal{T}_{-1}] + [\mathcal{T}'_1,\mathcal{T}_0] + [\mathcal{T}_0,\mathcal{T}'_{-1}]\right) + \mathrm{O}\left((1/U)^2\right),\end{aligned} \quad \text{(E.15)}$$

where we used the following relations:

$$\begin{aligned}[\mathrm{i}\mathcal{S}^{(1)},\mathcal{H}] &= -(\mathcal{T}_1 + \mathcal{T}_{-1} + \mathcal{T}'_1 + \mathcal{T}'_{-1}) + \frac{2}{U}([\mathcal{T}_1,\mathcal{T}_{-1}] + [\mathcal{T}_1,\mathcal{T}'_{-1}] + [\mathcal{T}'_1,\mathcal{T}_{-1}] + [\mathcal{T}'_1,\mathcal{T}'_{-1}]) \\ &\quad + \frac{1}{U}([\mathcal{T}_1,\mathcal{T}_0] + [\mathcal{T}_0,\mathcal{T}_{-1}] + [\mathcal{T}'_1,\mathcal{T}_0] + [\mathcal{T}_0,\mathcal{T}'_{-1}]),\end{aligned} \quad \text{(E.16)}$$

$$[\mathrm{i}\mathcal{S}^{(1)},[\mathrm{i}\mathcal{S}^{(1)},\mathcal{H}]] = -\frac{2}{U}([\mathcal{T}_1,\mathcal{T}_{-1}] + [\mathcal{T}_1,\mathcal{T}'_{-1}] + [\mathcal{T}'_1,\mathcal{T}_{-1}] + [\mathcal{T}'_1,\mathcal{T}'_{-1}]) + \mathrm{O}\left((1/U)^2\right), \quad \text{(E.17)}$$

$$[\mathrm{i}\mathcal{S}^{(1)},[\mathrm{i}\mathcal{S}^{(1)},[\mathrm{i}\mathcal{S}^{(1)},\mathcal{H}]]] = \mathrm{O}\left((1/U)^2\right). \quad \text{(E.18)}$$

For the purpose of further procedures, we introduce the operator $\mathcal{T}^{(k)}(m_1, m_2, \cdots, m_k)$ of the form

$$\mathcal{T}^{(k)}(m_1, m_2, \cdots, m_k) \equiv \mathcal{T}^{(k)}[m] = \mathcal{T}_{m_1}\mathcal{T}_{m_2}\cdots\mathcal{T}_{m_k}. \quad \text{(E.19)}$$

We can easily derive the following relation by noting Eq. (E.10):

$$[\mathcal{V},\mathcal{T}^{(k)}[m]] = U\sum_{l=1}^{k} m_l\mathcal{T}^{(k)}[m] = UM^{(k)}[m]\mathcal{T}^{(k)}[m], \quad \text{(E.20)}$$

where we define $M^{(k)}[m]$ as

$$M^{(k)}[m] \equiv \sum_{l=1}^{k} m_l. \quad \text{(E.21)}$$

The transformed Hamiltonian $\mathcal{H}'^{(k)}$ in Eq. (E.12), by definition, does not have hopping terms that change the number of doubly occupied sites, in the order higher than $(1/U)^{k-2}$. It can have the following form:

$$\mathcal{H}'^{(k)} = \mathcal{V} + \sum_{l=1}^{k-1} U^{1-l} \sum_{\{m|M[m]=0\}} C^{(l)}[m]\mathcal{T}^{(l)}[m] + U^{1-k}\sum_{\{m\}} C^{(k)}[m]\mathcal{T}^{(k)}[m] + \mathrm{O}\left((1/U)^k\right), \quad \text{(E.22)}$$

where $C^{(k)}[m]$ is a parameter. We here prove that we can eliminate all of the terms that change the number of doubly occupied sites, in the order $(1/U)^{k-1}$ by choosing $\mathrm{i}\mathcal{S}^{(k)}$ as

$$\mathrm{i}\mathcal{S}^{(k)} \equiv U^{-k}\sum_{\{m|M[m]\neq 0\}} \frac{C^{(k)}[m]\mathcal{T}^{(k)}[m]}{M^{(k)}[m]}. \quad \text{(E.23)}$$

The transformed Hamiltonian $\mathcal{H}'^{(k+1)}$ is produced in the following procedure:

$$\mathcal{H}'^{(k+1)} = e^{\mathrm{i}\mathcal{S}^{(k)}}\mathcal{H}'^{(k)}e^{-\mathrm{i}\mathcal{S}^{(k)}} = \mathcal{H}'^{(k)} + [\mathrm{i}\mathcal{S}^{(k)},\mathcal{H}'^{(k)}] + \frac{[\mathrm{i}\mathcal{S}^{(k)},[\mathrm{i}\mathcal{S}^{(k)},\mathcal{H}'^{(k)}]]}{2} + \cdots. \quad \text{(E.24)}$$

The term $[\mathrm{i}\mathcal{S}^{(k)}, \mathcal{H}'^{(k)}]$ is given by

$$
\begin{aligned}
&[\mathrm{i}\mathcal{S}^{(k)}, \mathcal{H}'^{(k)}] \\
&= [\mathrm{i}\mathcal{S}^{(k)}, \mathcal{V} + \sum_{l=1}^{k-1} U^{1-l} \sum_{\{m|M[m]=0\}} C^{(l)}[m]\mathcal{T}^{(l)}[m] + U^{1-k} \sum_{\{m\}} C^{(k)}[m]\mathcal{T}^{(k)}[m] + \mathrm{O}\left((1/U)^k\right)] \\
&= [\mathrm{i}\mathcal{S}^{(k)}, \mathcal{V}] + \mathrm{O}\left((1/U)^k\right), \qquad \text{(E.25)}
\end{aligned}
$$

where

$$
\begin{aligned}
&[\mathrm{i}\mathcal{S}^{(k)}, \mathcal{V}] = U^{-k} \sum_{\{m|M[m]\neq 0\}} \frac{C^{(k)}[m]}{M^{(k)}[m]}[\mathcal{T}^{(k)}[m], \mathcal{V}] \\
=&U^{-k} \sum_{\{m|M[m]\neq 0\}} \frac{C^{(k)}[m]}{M^{(k)}[m]} \left(-UM^{(k)}[m]\mathcal{T}^{(k)}[m]\right) = -U^{1-k} \sum_{\{m|M[m]\neq 0\}} C^{(k)}[m]\mathcal{T}^{(k)}[m]. \qquad \text{(E.26)}
\end{aligned}
$$

By noting

$$
[\mathrm{i}\mathcal{S}^{(k)}, [\mathrm{i}\mathcal{S}^{(k)}, \mathcal{H}'^{(k)}]] = \mathrm{O}\left((1/U)^{2k-1}\right), \qquad \text{(E.27)}
$$

we obtain

$$
\begin{aligned}
\mathcal{H}'^{(k+1)} =& e^{\mathrm{i}\mathcal{S}^{(k)}} \mathcal{H}'^{(k)} e^{-\mathrm{i}\mathcal{S}^{(k)}} = \mathcal{H}'^{(k)} + [\mathrm{i}\mathcal{S}^{(k)}, \mathcal{H}'^{(k)}] + \frac{[\mathrm{i}\mathcal{S}^{(k)}, [\mathrm{i}\mathcal{S}^{(k)}, \mathcal{H}'^{(k)}]]}{2} + \cdots \\
=& \mathcal{V} + \sum_{l=1}^{k-1} U^{1-l} \sum_{\{m|M[m]=0\}} C^{(l)}[m]\mathcal{T}^{(l)}[m] + U^{1-k} \sum_{\{m\}} C^{(k)}[m]\mathcal{T}^{(k)}[m] \\
&- U^{1-k} \sum_{\{m|M[m]\neq 0\}} C^{(k)}[m]\mathcal{T}^{(k)}[m] + \mathrm{O}\left((1/U)^k\right) \\
=& \mathcal{V} + \sum_{l=1}^{k} U^{1-l} \sum_{\{m|M[m]=0\}} C^{(l)}[m]\mathcal{T}^{(l)}[m] + \mathrm{O}\left((1/U)^k\right). \qquad \text{(E.28)}
\end{aligned}
$$

We therefore confirm that we can eliminate the terms of order $(1/U)^{k-1}$ in Eq. (E.22) by operating $e^{\mathrm{i}\mathcal{S}^{(k)}}$ and $e^{-\mathrm{i}\mathcal{S}^{(k)}}$ to $\mathcal{H}'^{(k)}$.

By using the expression (E.23) and by referring to Eq. (E.15), we have $\mathrm{i}\mathcal{S}^{(2)}$ as

$$
\mathrm{i}\mathcal{S}^{(2)} = U^{-2} \sum_{\{m|M[m]\neq 0\}} \frac{C^{(2)}[m]\mathcal{T}^{(2)}[m]}{M^{(2)}[m]} = \frac{1}{U^2}([\mathcal{T}_1, \mathcal{T}_0] - [\mathcal{T}_0, \mathcal{T}_{-1}] + [\mathcal{T}_1', \mathcal{T}_0] - [\mathcal{T}_0, \mathcal{T}_{-1}']). \qquad \text{(E.29)}
$$

We thus obtain $\mathcal{H}'^{(3)}$ in the form:

$$\begin{aligned}
\mathcal{H}'^{(3)} &= e^{\mathrm{i}\mathcal{S}^{(2)}}\mathcal{H}'^{(2)}e^{-\mathrm{i}\mathcal{S}^{(2)}} = \mathcal{H}'^{(2)} + [\mathrm{i}\mathcal{S}^{(2)}, \mathcal{H}'^{(2)}] + \frac{[\mathrm{i}\mathcal{S}^{(2)}, [\mathrm{i}\mathcal{S}^{(2)}, \mathcal{H}'^{(2)}]]}{2} + \cdots \\
&= \mathcal{V} + \mathcal{T}_0 + \frac{1}{U}\left([\mathcal{T}_1, \mathcal{T}_{-1}] + [\mathcal{T}_1, \mathcal{T}'_{-1}] + [\mathcal{T}'_1, \mathcal{T}_{-1}] + [\mathcal{T}'_1, \mathcal{T}'_{-1}]\right. \\
&\quad \left. +[\mathcal{T}_1, \mathcal{T}_0] + [\mathcal{T}_0, \mathcal{T}_{-1}] + [\mathcal{T}'_1, \mathcal{T}_0] + [\mathcal{T}_0, \mathcal{T}'_{-1}]\right) \\
&\quad + \frac{1}{U^2}\left[([\mathcal{T}_1, \mathcal{T}_0] - [\mathcal{T}_0, \mathcal{T}_{-1}] + [\mathcal{T}'_1, \mathcal{T}_0] - [\mathcal{T}_0, \mathcal{T}'_{-1}]), \mathcal{V}\right] + \mathrm{O}\left((1/U)^2\right) \\
&= \mathcal{V} + \mathcal{T}_0 + \frac{1}{U}\left([\mathcal{T}_1, \mathcal{T}_{-1}] + [\mathcal{T}_1, \mathcal{T}'_{-1}] + [\mathcal{T}'_1, \mathcal{T}_{-1}] + [\mathcal{T}'_1, \mathcal{T}'_{-1}]\right) + \mathrm{O}\left((1/U)^2\right).
\end{aligned} \tag{E.30}$$

E.2 Effective Hamiltonian in the half-filled case

We consider the Hamiltonian (E.30) in the half-filled case. We restrict ourselves to the subspace where there are no doubly occupied sites. For any basis $|\Psi_L\rangle$ in our subspace, the relations

$$\mathcal{T}_{-1}|\Psi_L\rangle = 0, \qquad \mathcal{T}'_{-1}|\Psi_L\rangle = 0 \tag{E.31}$$

must be satisfied. Equation (E.31) is generalized in the form

$$\mathcal{T}^{(k)}[m]|\Psi_L\rangle \equiv 0 \tag{E.32}$$

for any integer n $(1 \leq n \leq k)$ as long as

$$M_n^{(k)}[m] \equiv \sum_{l=n}^{k} m_l < 0. \tag{E.33}$$

The Hamiltonian $\mathcal{H}'^{(3)}$ in Eq. (E.30) is then reduced in the subspace to

$$\mathcal{H}'^{(3)}_{\mathrm{HL}} = \mathcal{V} + \mathcal{T}_0 - \frac{1}{U}\left(\mathcal{T}_{-1}\mathcal{T}_1 + \mathcal{T}'_{-1}\mathcal{T}_1 + \mathcal{T}_{-1}\mathcal{T}'_1 + \mathcal{T}'_{-1}\mathcal{T}'_1\right) + \mathrm{O}\left((1/U)^2\right). \tag{E.34}$$

By noting

$$\mathcal{V}|\Psi_L\rangle = 0, \quad \mathcal{T}_0|\Psi_L\rangle = 0, \quad \mathcal{T}'_{-1}\mathcal{T}_1|\Psi_L\rangle = 0, \quad \mathcal{T}_{-1}\mathcal{T}'_1|\Psi_L\rangle = 0, \tag{E.35}$$

we arrive at the Hamiltonian $\mathcal{H}'^{(3)}_{\mathrm{HL}}$ of the form

$$\mathcal{H}'^{(3)}_{\mathrm{HL}} = -\frac{1}{U}\left(\mathcal{T}_{-1}\mathcal{T}_1 + \mathcal{T}'_{-1}\mathcal{T}'_1\right) + \mathrm{O}\left((1/U)^2\right). \tag{E.36}$$

Specifically, the Hamiltonian $\mathcal{H}'^{(3)}_{\mathrm{HL}}$ is given by

$$
\begin{aligned}
\mathcal{H}'^{(3)}_{\mathrm{HL}} = &-\frac{t^2}{U}\sum_{i_1,i_2=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}\Big((e^{g\sigma_1}h_{i_1+1,\bar{\sigma_1}}c^{\dagger}_{i_1+1,\sigma_1}c_{i_1,\sigma_1}n_{i_1,\bar{\sigma_1}}+e^{-g\sigma_1}h_{i_1,\bar{\sigma_1}}c^{\dagger}_{i_1,\sigma_1}c_{i_1+1,\sigma_1}n_{i_1+1,\bar{\sigma_1}})\\
&\times(e^{g\sigma_2}n_{i_2+1,\bar{\sigma_2}}c^{\dagger}_{i_2+1,\sigma_2}c_{i_2,\sigma_2}h_{i_2,\bar{\sigma_2}}+e^{-g\sigma_2}n_{i_2,\bar{\sigma_2}}c^{\dagger}_{i_2,\sigma_2}c_{i_2+1,\sigma_2}h_{i_2+1,\bar{\sigma_2}})\Big)\\
&-\frac{t'^2}{U}\sum_{i_1,i_2=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}\Big((e^{2g\sigma_1}h_{i_1+2,\bar{\sigma_1}}c^{\dagger}_{i_1+2,\sigma_1}c_{i_1,\sigma_1}n_{i_1,\bar{\sigma_1}}+e^{-2g\sigma_1}h_{i_1,\bar{\sigma_1}}c^{\dagger}_{i_1,\sigma_1}c_{i_1+2,\sigma_1}n_{i_1+2,\bar{\sigma_1}})\\
&\times(e^{2g\sigma_2}n_{i_2+2,\bar{\sigma_2}}c^{\dagger}_{i_2+2,\sigma_2}c_{i_2,\sigma_2}h_{i_2,\bar{\sigma_2}}+e^{-2g\sigma_2}n_{i_2,\bar{\sigma_2}}c^{\dagger}_{i_2,\sigma_2}c_{i_2+2,\sigma_2}h_{i_2+2,\bar{\sigma_2}})\Big)+\mathrm{O}\left((1/U)^2\right).
\end{aligned}
\tag{E.37}
$$

In order to prohibit doubly occupied sites and empty sites, the relation $i_1 = i_2$ must be satisfied. We thus rewrite Eq. (E.37) as follows:

$$
\begin{aligned}
\mathcal{H}'^{(3)}_{\mathrm{HL}} = & -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+1,\bar{\sigma}_1}c^{\dagger}_{i+1,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i+1,\bar{\sigma}_2}c^{\dagger}_{i+1,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{g(\sigma_1+\sigma_2)}}_{\mathcal{A}_1} \\
& -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+1,\bar{\sigma}_1}c^{\dagger}_{i+1,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+1,\sigma_2}h_{i+1,\bar{\sigma}_2})e^{g(\sigma_1-\sigma_2)}}_{\mathcal{A}_2} \\
& -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+1,\sigma_1}n_{i+1,\bar{\sigma}_1}n_{i+1,\bar{\sigma}_2}c^{\dagger}_{i+1,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{g(-\sigma_1+\sigma_2)}}_{\mathcal{A}_3} \\
& -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+1,\sigma_1}n_{i+1,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+1,\sigma_2}h_{i+1,\bar{\sigma}_2})e^{-g(\sigma_1+\sigma_2)}}_{\mathcal{A}_4} \\
& -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+2,\bar{\sigma}_1}c^{\dagger}_{i+2,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i+2,\bar{\sigma}_2}c^{\dagger}_{i+2,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{2g(\sigma_1+\sigma_2)}}_{\mathcal{A}_5} \\
& -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+2,\bar{\sigma}_1}c^{\dagger}_{i+2,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+2,\sigma_2}h_{i+2,\bar{\sigma}_2})e^{2g(\sigma_1-\sigma_2)}}_{\mathcal{A}_6} \\
& -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+2,\sigma_1}n_{i+2,\bar{\sigma}_1}n_{i+2,\bar{\sigma}_2}c^{\dagger}_{i+2,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{2g(-\sigma_1+\sigma_2)}}_{\mathcal{A}_7} \\
& -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+2,\sigma_1}n_{i+2,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+2,\sigma_2}h_{i+2,\bar{\sigma}_2})e^{-2g(\sigma_1+\sigma_2)}}_{\mathcal{A}_8}.
\end{aligned}
\tag{E.38}
$$

Since the basis $|\Psi_L\rangle$ have no doubly occupied sites, the relations

$$
\mathcal{A}_1|\Psi_L\rangle = 0, \quad \mathcal{A}_4|\Psi_L\rangle = 0, \quad \mathcal{A}_5|\Psi_L\rangle = 0, \quad \mathcal{A}_8|\Psi_L\rangle = 0, \tag{E.39}
$$

must be satisfied. By using (E.39), $\mathcal{H}'^{(3)}_{\mathrm{HL}}$ in Eq. (E.38) becomes

$$\begin{aligned}\mathcal{H}'^{(3)}_{\mathrm{HL}} =& -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+1,\bar{\sigma}_1}c^{\dagger}_{i+1,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+1,\sigma_2}h_{i+1,\bar{\sigma}_2})e^{g(\sigma_1-\sigma_2)}}_{\mathcal{A}_2} \\ & -\frac{t^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+1,\sigma_1}n_{i+1,\bar{\sigma}_1}n_{i+1,\bar{\sigma}_2}c^{\dagger}_{i+1,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{g(-\sigma_1+\sigma_2)}}_{\mathcal{A}_3} \\ & -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i+2,\bar{\sigma}_1}c^{\dagger}_{i+2,\sigma_1}c_{i,\sigma_1}n_{i,\bar{\sigma}_1}n_{i,\bar{\sigma}_2}c^{\dagger}_{i,\sigma_2}c_{i+2,\sigma_2}h_{i+2,\bar{\sigma}_2})e^{2g(\sigma_1-\sigma_2)}}_{\mathcal{A}_6} \\ & -\frac{t'^2}{U}\underbrace{\sum_{i=1}^{L}\sum_{\sigma_1,\sigma_2=\uparrow,\downarrow}(h_{i,\bar{\sigma}_1}c^{\dagger}_{i,\sigma_1}c_{i+2,\sigma_1}n_{i+2,\bar{\sigma}_1}n_{i+2,\bar{\sigma}_2}c^{\dagger}_{i+2,\sigma_2}c_{i,\sigma_2}h_{i,\bar{\sigma}_2})e^{2g(-\sigma_1+\sigma_2)}}_{\mathcal{A}_7}.\end{aligned} \tag{E.40}$$

By noting that all $|\Psi_L\rangle$ satisfy $n_{i,\uparrow}+n_{i,\downarrow}=1$ and by using the transformation

$$S^+_i = c^{\dagger}_{i,\uparrow}c_{i,\downarrow}, \quad S^-_i = c^{\dagger}_{i,\downarrow}c_{i,\uparrow}, \quad S^z_i = \frac{1}{2}(n_{i,\uparrow}-n_{i,\downarrow}), \tag{E.41}$$

we have $\mathcal{A}_2$ and $\mathcal{A}_3$ in the forms

$$\mathcal{A}_2 = \mathcal{A}_3 = -\sum_{i=1}^{L}\left[e^{2g}S^+_{i+1}S^-_i + e^{-2g}S^+_iS^-_{i+1} + 2S^z_iS^z_{i+1} - \frac{1}{2}\right] \tag{E.42}$$

after some algebra. We next calculate $\mathcal{A}_6$ and $\mathcal{A}_7$ in the same procedure:

$$\mathcal{A}_6 = \mathcal{A}_7 = -\sum_{i=1}^{L}\left[e^{4g}S^+_{i+2}S^-_i + e^{-4g}S^+_iS^-_{i+2} + 2S^z_iS^z_{i+2} - \frac{1}{2}\right]. \tag{E.43}$$

We thus obtain the effective Hamiltonian of the non-Hermitian t-t'-U model of the form

$$\begin{aligned}\mathcal{H}'^{(3)}_{\mathrm{HL}} =& \frac{4t^2}{U}\sum_{i=1}^{L}\left[\frac{1}{2}\left(e^{2g}S^+_{i+1}S^-_i + e^{-2g}S^+_iS^-_{i+1}\right) + S^z_iS^z_{i+1} - \frac{1}{4}\right] \\ & + \frac{4t'^2}{U}\sum_{i=1}^{L}\left[\frac{1}{2}\left(e^{4g}S^+_{i+2}S^-_i + e^{-4g}S^+_iS^-_{i+2}\right) + S^z_iS^z_{i+2} - \frac{1}{4}\right].\end{aligned} \tag{E.44}$$

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