Master Thesis

Nontrivial complex eigenvalues of the Liouvillian in open quantum systems

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January 12, 2011

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Contents

Abstract

We solve the eigenvalue problem of the Liouvilian of an open quantum system by perturbation analysis. Our model consists of a dot and an infinitely long lead. We find complex eigenvalues that cannot be predicted from the eigenvalues of the corresponding Hamiltonian, by expanding the domain of the Green's function. We expect that a nontrivial complex eigenvalue describes the relaxation time from a quasi-stable state to the equilibrium state.

We also introduce the method of obtaining the eigenvalues of the Liouvillian rigorously. The core of this method is the fact that the eigenvalue problem of a one-particle Liouvillian is reduced to that of a two-particle Hamiltonian. In our model, though the original model does not have the two-body interaction, the two-particle Hamiltonian mapped from the original problem has a two-body interaction. This suggests the existence of the nontrivial eigenvalues of the original Liouvillian.

This thesis is based on the paper [1].

Chapter 1

Introduction

If a system has a compact potential in an infinite volume, we can obtain complex eigenvalues of the Hamiltonian under the boundary conditions of outgoing waves only or incoming waves only [2, 3], or with the Feshbach formalism (see Appendix A.1) [4, 5]. The eigenstates corresponding to the complex eigenvalues are not ghost states but have physical meaning; they describe resonance states, which play crucial roles in high-energy physics, and the imaginary part of the complex eigenvalues is the inverse lifetime of the corresponding resonance state [3, 6–23], though they do not have probabilistic interpretation because of divergence of their norms. (See, however, Ref. [2] for an extended probabilistic interpretation.)

A discussion of the same sort can be applied to the Liouvillian, which is the generator of the time evolution of density matrices in the Liouville-von Neumann equation:

$$i\frac{\partial}{\partial t}\rho = L\rho = [H, \rho], \tag{1.1}$$

where we use the unit with $\hbar = 1$. In the infinite system with a compact potential, we expect that the Liouvillian can have complex eigenvalues z as in $L\rho = z\rho$ under certain boundary conditions, which have not been yet understood well, nor with the Feshbach formalism for the Liouville operator. For finite systems, all the eigenvectors and the eigenvalues of the Liouvillian are written in the forms $\rho_{nm} = |n\rangle\langle m|$ and $z_{nm} = E_n - E_m$, respectively, where $|n\rangle$ and E_n are a discrete eigenstate and its eigenvalue of the corresponding Hamiltonian, respectively. For infinite systems, on the other hand, the discrete eigenvalues of the Liouvillian may be of two types: one is $z_{\alpha\beta} = E_\alpha - E_\beta$, where α and β are indices of discrete eigenvalues of the corresponding Hamiltonian including their complex eigenvalues, and the other is the type not written in the form $E_\alpha - E_\beta$, which we call nontrivial eigenvalues. An example of the nontrivial eigenvalue for the one-dimensional quantum gas interacting by the delta function potential has been discussed on the level of the weak-coupling approximation [24]. They showed that the nontrivial part of the eigenvalue gives a transport coefficient of the system. In contrast, we here present [1] a method without any approximation of finding nontrivial eigenvalues of the Liouvillian of open quantum systems in sec. 3.1 and perturbation analysis of another model in sec. 2.4.

The reason why we are interested in such eigenvalues is that the eigenstates corresponding to them may include physically relevant non-equilibrium states and the imaginary part of the eigenvalue can be the inverse relaxation time. In contrast to finite

systems, infinite systems have dissipation of particles into the infinity. Therefore, a state with relaxation can be an eigenstate of the Liouvillian under appropriate boundary conditions. Its eigenvalue may be complex and the corresponding eigenstate may be of the form $\sum_{\alpha,\beta} c_{\alpha\beta}|\alpha\rangle\langle\beta|$ with some coefficients $c_{\alpha\beta}$. We can find such a state not by analyzing the Hamiltonian, but only by analyzing the Liouvillian.

The thesis is organized as follows. In Chap. 2, we solve the eigenvalues of the Liouvillian by the perturbation analysis. In Sec. 2.1, we introduce the model and the approach. In Sec. 2.2, we introduce our diagram expansion and show the evidence for the existence of the nontrivial eigenvalues of the Liouvillian by indicating the simultaneous operation of a Green's-function operator on the bra state and ket state. In Sec. 2.3, we show how to obtain the integral equation corresponding to the eigenvalue problem of the Liouvillian. In Sec. 2.4, we obtain trivial and nontrivial eigenvalues by the second-order perturbation analysis of the integral equation. In Chap. 3, we introduce the method of solving the eigenvalue problem of the Liouvillian rigorously. In Sec. 3.1, we show the powerfulness of this method by expanding the model that we treat. In Sec. 3.2, using this method we try to obtain the eigenvalues of the Liouvillian rigorously. It is not a simple calculation, and unfortunately we do not arrive at the final solution. However, this method may be an easy methodology of obtaining the relaxation time.

Chapter 2

Perturbation analysis

2.1 Model and approach

Let us introduce the system that we consider. We analyze an open quantum system, where the particle can dissipate into the infinity. A T-type quantum dot with an infinitely long lead (Fig. 2.1) is the simplest model that has the above properties: the potential is compact whereas the volume is infinite. The Hamiltonian is given by the following:

$$H = -t \sum_{x=-\infty}^{\infty} (c_{x+1}^{\dagger} c_x + c_x^{\dagger} c_{x+1}) + (-t_1)(d^{\dagger} c_0 + c_0^{\dagger} d), \tag{2.1}$$

where $c_x^{\dagger}$ and c_x are the creation and annihilation operators at the site x on the lead, while $d^{\dagger}$ and d are those at the dot site. We can rigorously obtain the spectrum of H including complex eigenvalues (see Appendix A.1). In particular, the Hamiltonian has complex eigenvalues under the boundary conditions of out-going waves only or in-coming waves only.

Our aim is to solve the eigenvalue problem of the corresponding Liouvillian:

$$L\rho = [H, \rho] = z\rho \tag{2.2}$$

under appropriate boundary conditions for obtaining complex eigenvalues z. We employ the Feshbach formalism [4, 5] (see Appendix A.1), which was originally developed for the eigenvalue problem of Hamiltonians. For the purpose, we next define the projection

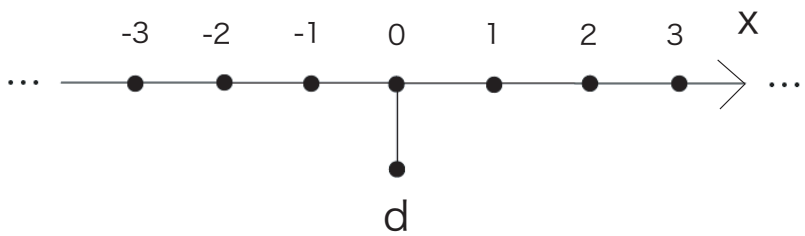

Figure 2.1: The T-type quantum dot with an infinite lead.

operators P and Q in the Liouville space as follows:

$$
\begin{aligned}
P &:= P_{\rm s} \times P_{\rm s}, && (2.3)\\
Q &:= Q_{\rm s} \times Q_{\rm s} + P_{\rm s} \times Q_{\rm s} + Q_{\rm s} \times P_{\rm s}, && (2.4)\\
P &+ Q = I, && (2.5)\\
& && (2.6)
\end{aligned}
$$

where the operation '$\times$' is defined in Appendix A.3 and the projection operators $P_{\rm s}$ and $Q_{\rm s}$ in the Hilbert space is defined for the system (2.1) as

$$P_{\rm s} = |d\rangle\langle d|, \tag{2.7}$$

$$Q_{\rm s} = \sum_{x=-\infty}^{\infty} |x\rangle\langle x|, \tag{2.8}$$

and thereby we have

$$P_{\rm s} + Q_{\rm s} = I_{\rm s}, \tag{2.9}$$

$$P_{\rm s} H P_{\rm s} = 0, \tag{2.10}$$

$$P_{\rm s} H Q_{\rm s} = -t_1 d^\dagger c_0, \tag{2.11}$$

$$Q_{\rm s} H P_{\rm s} = -t_1 c_0^\dagger d, \tag{2.12}$$

$$Q_{\rm s} H Q_{\rm s} = -t \sum_{x=-\infty}^{\infty} (c_{x+1}^\dagger c_x + c_x^\dagger c_{x+1}), \tag{2.13}$$

where $I_{\rm s}$ is the identity operator in the Hilbert space. Then, the Feshbach formalism transforms Eq. (2.2) in the form

$$L_{\rm eff}(z)(P\rho) = z(P\rho), \tag{2.14}$$

where

$$L_{\rm eff}(z) = PLP + PLQ\frac{1}{z - QLQ}QLP. \tag{2.15}$$

For the system (2.1), the eigenvalue problem (2.2) therefore reduces to

$$\langle\langle d, d|L_{\rm eff}(z)|d, d\rangle\rangle = z, \tag{2.16}$$

where

$$|d, d\rangle\rangle := |d\rangle\langle d| = d^\dagger|{\rm vac}\rangle\langle{\rm vac}|d, \tag{2.17}$$

$$|d, 0\rangle\rangle := |d\rangle\langle 0| = d^\dagger|{\rm vac}\rangle\langle{\rm vac}|c_0, \tag{2.18}$$

and so on, with $|{\rm vac}\rangle$ being the vacuum state. We obtained Eq. (2.16) because the operator $P = P_{\rm s} \times P_{\rm s}$ projects everything on the state $|d, d\rangle\rangle = |d\rangle\langle d|$. We have

$$
\begin{aligned}
PLP &= (P_{\rm s} \times P_{\rm s})(H \times I_{\rm s} - I_{\rm s} \times H)(P_{\rm s} \times P_{\rm s})\\
&= P_{\rm s} H P_{\rm s} \times P_{\rm s} - P_{\rm s} \times P_{\rm s} H P_{\rm s} = 0 && (2.19)
\end{aligned}
$$

because of Eq. (2.10). The other terms in Eq. (2.15) are given as follows;

$$
\begin{aligned}
PLQ &= (P_{\rm s}\times P_{\rm s})\,(H\times I_{\rm s}-I_{\rm s}\times H)\,(Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\\
&= (P_{\rm s}H\times P_{\rm s}-P_{\rm s}\times HP_{\rm s})\,(Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\\
&= P_{\rm s}HQ_{\rm s}\times P_{\rm s}-P_{\rm s}\times Q_{\rm s}HP_{\rm s}, \qquad (2.20)\\
QLP &= (Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\,(H\times I_{\rm s}-I_{\rm s}\times H)\,(P_{\rm s}\times P_{\rm s})\\
&= (Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\,(HP_{\rm s}\times P_{\rm s}-P_{\rm s}\times P_{\rm s}H)\\
&= Q_{\rm s}HP_{\rm s}\times P_{\rm s}-P_{\rm s}\times P_{\rm s}HQ_{\rm s}, \qquad (2.21)\\
QLQ &= (Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\,(H\times I_{\rm s}-I_{\rm s}\times H)\,(Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\\
&= (Q_{\rm s}H\times P_{\rm s}+P_{\rm s}H\times Q_{\rm s}+Q_{\rm s}H\times Q_{\rm s}-Q_{\rm s}\times HP_{\rm s}-P_{\rm s}\times HQ_{\rm s}-Q_{\rm s}\times HQ_{\rm s})\\
&\quad (Q_{\rm s}\times P_{\rm s}+P_{\rm s}\times Q_{\rm s}+Q_{\rm s}\times Q_{\rm s})\\
&= Q_{\rm s}HQ_{\rm s}\times P_{\rm s}+P_{\rm s}HP_{\rm s}\times Q_{\rm s}+P_{\rm s}HQ_{\rm s}\times Q_{\rm s}+Q_{\rm s}HP_{\rm s}\times Q_{\rm s}+Q_{\rm s}HQ_{\rm s}\times Q_{\rm s}\\
&- Q_{\rm s}\times P_{\rm s}HP_{\rm s}-Q_{\rm s}\times Q_{\rm s}HP_{\rm s}-P_{\rm s}\times Q_{\rm s}HQ_{\rm s}-Q_{\rm s}\times P_{\rm s}HQ_{\rm s}-Q_{\rm s}\times Q_{\rm s}HQ_{\rm s}\\
&= Q_{\rm s}HQ_{\rm s}\times 1+P_{\rm s}HP_{\rm s}\times Q_{\rm s}+P_{\rm s}HQ_{\rm s}\times Q_{\rm s}+Q_{\rm s}HP_{\rm s}\times Q_{\rm s}\\
&- 1\times Q_{\rm s}HQ_{\rm s}-Q_{\rm s}\times P_{\rm s}HP_{\rm s}-Q_{\rm s}\times Q_{\rm s}HP_{\rm s}-Q_{\rm s}\times P_{\rm s}HQ_{\rm s}\\
&= Q_{\rm s}HQ_{\rm s}\times 1+P_{\rm s}HQ_{\rm s}\times Q_{\rm s}+Q_{\rm s}HP_{\rm s}\times Q_{\rm s}\\
&- 1\times Q_{\rm s}HQ_{\rm s}-Q_{\rm s}\times Q_{\rm s}HP_{\rm s}-Q_{\rm s}\times P_{\rm s}HQ_{\rm s}, \qquad (2.22)
\end{aligned}
$$

where we again used $P_{\rm s}HP_{\rm s}=0$.

Then, the element $\langle\langle d,d|L_{\rm eff}|d,d\rangle\rangle$ on the left-hand side of Eq. (2.16) is given as follows:

$$
\begin{aligned}
\langle\langle d,d|L_{\rm eff}(z)|d,d\rangle\rangle &= t_1^2\langle\langle d,0|\frac{1}{z-QLQ}|d,0\rangle\rangle - t_1^2\langle\langle d,0|\frac{1}{z-QLQ}|0,d\rangle\rangle\\
&\quad -t_1^2\langle\langle 0,d|\frac{1}{z-QLQ}|d,0\rangle\rangle + t_1^2\langle\langle 0,d|\frac{1}{z-QLQ}|0,d\rangle\rangle. \qquad (2.23)
\end{aligned}
$$

The equation to be solved is given as follows:

$$
\begin{aligned}
z &= t_1^2\langle\langle d,0|\frac{1}{z-QLQ}|d,0\rangle\rangle - t_1^2\langle\langle d,0|\frac{1}{z-QLQ}|0,d\rangle\rangle\\
&\quad - t_1^2\langle\langle 0,d|\frac{1}{z-QLQ}|d,0\rangle\rangle + t_1^2\langle\langle 0,d|\frac{1}{z-QLQ}|0,d\rangle\rangle. \qquad (2.24)
\end{aligned}
$$

As we see in the above equation, the problem of analyzing Eq. (2.15) is reduced to obtaining the Green's function of the partial Liouvillian QLQ given in Eq. (2.22).

2.2 Diagram expansion

In the present section, we show a sign of the existence of the nontrivial eigenvalues, which is not of the type of $E_\alpha - E_\beta$, by describing the diagram expansion of the Green's function of QLQ in Eq. (2.24).

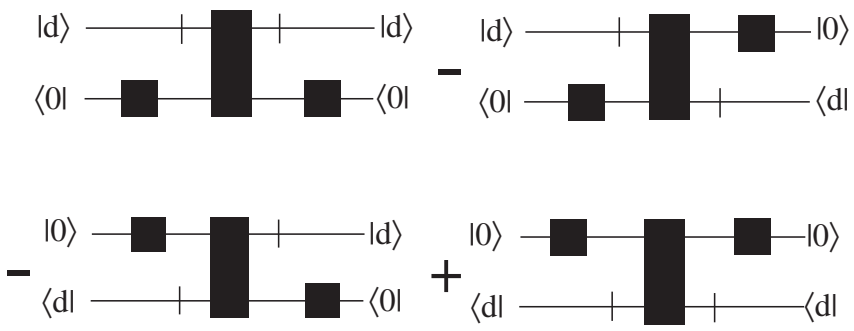

Figure 2.2: The diagrams for the term $n = 2$ of the expansion (2.30).

We first divide the partial Liouvillian QLQ into the following two parts:

$$QLQ = L_0 + L_1, \tag{2.25}$$

$$L_0 = Q_{\mathrm{s}} H Q_{\mathrm{s}} \times I_{\mathrm{s}} - I_{\mathrm{s}} \times Q_{\mathrm{s}} H Q_{\mathrm{s}}, \tag{2.26}$$

$$\begin{aligned} L_1 =& Q_{\mathrm{s}} H P_{\mathrm{s}} \times Q_{\mathrm{s}} - Q_{\mathrm{s}} \times P_{\mathrm{s}} H Q_{\mathrm{s}} \\ &+ P_s H Q_s \times Q_s - Q_s \times Q_s H P_s. \end{aligned} \tag{2.27}$$

We then define the Green's functions G and G_0 as follows:

$$G = \frac{1}{z - QLQ}, \tag{2.28}$$

$$G_0 = \frac{1}{z - L_0}. \tag{2.29}$$

Then we obtain

$$G = G_0 \sum_{n=0}^{\infty} (L_1 G_0)^n, \tag{2.30}$$

using the resolvent expansion.

Hereafter, we introduce our diagram exemplified in Fig. 2.2:

- The upper line shows the time evolution of the bra state.
- The lower line shows the time evolution of the ket state.
- A thin vertical line indicates the action of L_1, which moves the particle from the lead to the dot or from the dot to the lead by one step.
- A square indicates the action of G_0.

Considering that the necessary elements of G are those in Eq. (2.23), we can describe the term $n = 2$ of the expansion (2.30) as in Fig. 2.2. Since G_0 is the Green's function of L_0, it can act only when the bra state or the ket state is in the Q_s space. In each diagram in Fig. 2.2, therefore, the squares appear only on the upper line or on the lower line when adjacent to the initial or final states. Once L_1 acts on a state in the P_s space, the state jumps from the P_s space to the Q_s space. Then G_0 can act on the upper and lower lines simultaneously. The fact that the Green's function G_0, which has information that the system has an infinite volume, acts on the bra state and the ket state simultaneously suggests the existence of the nontrivial eigenvalues which cannot be described as $E_\alpha - E_\beta$.

2.3 Integral equation

In the present section, we show that obtaining the elements of the Green's function of QLQ is equivalent to solving two simultaneous integral equations.

The Dyson equation up to the second order reads

$$G = G_0 + G_0 L_1 G_0 L_1 G, \tag{2.31}$$

where the first-order term $G_0 L_1 G_0$ vanishes because of the following reason. We will need the matrix elements of G between $\langle\langle x, d|$ or $\langle\langle d, x|$ and $|0, d\rangle\rangle$ or $|d, 0\rangle\rangle$. In other words, one of the bra and ket states is in the P_s space while the other is in the Q_s space, both in the initial and final states. However, the operator L_1 moves either a state in the P_s space to the Q_s space or one in the Q_s space to the P_s space. Therefore, after operating L_1 on the initial state an odd number of times, both of the bra and ket states are in the same space. Such a state cannot have a matrix element with the final state. Therefore all the odd terms vanish.

For the matrix elements given in Eq. (2.23), we obtain the following relations using the closure introduced in Appendix A.3:

$$\begin{aligned}
\langle\langle x, d|G|0, d\rangle\rangle &= \langle\langle x, d|G_0|0, d\rangle\rangle \\
&\quad + \sum_{x_1, x_2, x_3} \langle\langle x, d|G_0|x_1, d\rangle\rangle \langle\langle x_1, d|L_1|x_1, 0\rangle\rangle \langle\langle x_1, 0|G_0|x_2, x_3\rangle\rangle \langle\langle x_2, x_3|L_1 G|0, d\rangle\rangle \\
&= \langle\langle x, d|G_0|0, d\rangle\rangle \\
&\quad + \sum_{x_1, x_2} \langle\langle x, d|G_0|x_1, d\rangle\rangle \langle\langle x_1, d|L_1|x_1, 0\rangle\rangle \langle\langle x_1, 0|G_0|x_2, 0\rangle\rangle \\
&\qquad \times \langle\langle x_2, 0|L_1|x_2, d\rangle\rangle \langle\langle x_2, d|G|0, d\rangle\rangle \\
&\quad + \sum_{x_1, x_3} \langle\langle x, d|G_0|x_1, d\rangle\rangle \langle\langle x_1, d|L_1|x_1, 0\rangle\rangle \langle\langle x_1, 0|G_0|0, x_3\rangle\rangle \\
&\qquad \times \langle\langle 0, x_3|L_1|d, x_3\rangle\rangle \langle\langle d, x_3|G|d, x\rangle\rangle \\
&= \langle\langle x, d|G_0|0, d\rangle\rangle \\
&\quad - t_1^2 \sum_{x_1, x_3} \langle\langle x, d|G_0|x_1, d\rangle\rangle \langle\langle x_1, 0|G_0|0, x_3\rangle\rangle \langle\langle d, x_3|G|0, d\rangle\rangle \\
&\quad + t_1^2 \sum_{x_1, x_2} \langle\langle x, d|G_0|x_1, d\rangle\rangle \langle\langle x_1, 0|G_0|x_2, 0\rangle\rangle \langle\langle x_2, d|G|0, d\rangle\rangle.
\end{aligned} \tag{2.32}$$

In the second equation, we used the property of L_1; the operator L_1 makes a particle take one step to the dot from the lead or to the lead from the dot. In the third equation, we replaced the matrix elements of L_1 with the hopping amplitude t_1. The other elements are similarly obtained as follows:

$$\begin{aligned}\langle\langle d,x|G|0,d\rangle\rangle &= t_1^2\sum_{x_1,x_3}\langle\langle d,x|G_0|d,x_1\rangle\rangle\langle\langle 0,x_1|G_0|0,x_3\rangle\rangle\langle\langle d,x_3|G|0,d\rangle\rangle \\ &\quad - t_1^2\sum_{x_1,x_2}\langle\langle d,x|G_0|d,x_1\rangle\rangle\langle\langle 0,x_1|G_0|x_2,0\rangle\rangle\langle\langle x_2,d|G|0,d\rangle\rangle, \end{aligned} \tag{2.33}$$

$$\begin{aligned}\langle\langle d,x|G|d,0\rangle\rangle &= \langle\langle d,x|G_0|d,0\rangle\rangle \\ &\quad + t_1^2\sum_{x_1,x_3}\langle\langle d,x|G_0|d,x_1\rangle\rangle\langle\langle 0,x_1|G_0|0,x_3\rangle\rangle\langle\langle d,x_3|G|d,0\rangle\rangle \\ &\quad - t_1^2\sum_{x_1,x_2}\langle\langle d,x|G_0|d,x_1\rangle\rangle\langle\langle 0,x_1|G_0|x_2,0\rangle\rangle\langle\langle x_2,d|G|d,0\rangle\rangle, \end{aligned} \tag{2.34}$$

$$\begin{aligned}\langle\langle x,d|G|d,0\rangle\rangle &= -t_1^2\sum_{x_1,x_3}\langle\langle x,d|G_0|x_1,d\rangle\rangle\langle\langle x_1,0|G_0|0,x_3\rangle\rangle\langle\langle d,x_3|G|d,0\rangle\rangle \\ &\quad + t_1^2\sum_{x_1,x_2}\langle\langle x,d|G_0|x_1,d\rangle\rangle\langle\langle x_1,0|G_0|x_2,0\rangle\rangle\langle\langle x_2,d|G|d,0\rangle\rangle. \end{aligned} \tag{2.35}$$

We rewrite Eqs. (2.32)–(2.35) with the Fourier transformation. We define the Fourier transformation of $\langle\langle x_1,x_2|L|x_3,x_4\rangle\rangle$ for an arbitrary operator L as follows:

$$\langle\langle x_1,x_2|L|x_3,x_4\rangle\rangle =: \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}e^{ik_1(x_1-x_3)}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}e^{-ik_2(x_2-x_4)}\hat{L}(k_1,k_2). \tag{2.36}$$

The Fourier elements $\hat{G}^{0d}(k;d)$ $\hat{G}^{0d}(d;k)$, $\hat{G}^{d0}(d;k)$ and $\hat{G}^{d0}(k;d)$ are also defined as follows:

$$\langle\langle x,d|G|0,d\rangle\rangle \equiv \int_{-\pi}^{\pi}\frac{dk}{2\pi}e^{ikx}\,\hat{G}^{0d}(k;d), \tag{2.37}$$

$$\langle\langle d,x|G|0,d\rangle\rangle \equiv \int_{-\pi}^{\pi}\frac{dk}{2\pi}e^{-ikx}\,\hat{G}^{0d}(d;k), \tag{2.38}$$

$$\langle\langle d,x|G|d,0\rangle\rangle \equiv \int_{-\pi}^{\pi}\frac{dk}{2\pi}e^{-ikx}\,\hat{G}^{d0}(d;k), \tag{2.39}$$

$$\langle\langle x,d|G|d,0\rangle\rangle \equiv \int_{-\pi}^{\pi}\frac{dk}{2\pi}e^{ikx}\,\hat{G}^{d0}(k;d). \tag{2.40}$$

Let us calculate the Green's function G_0 of $L_0 = Q_{\rm s}HQ_{\rm s}\times 1 - 1\times Q_{\rm s}HQ_{\rm s}$ using the Fourier transformation. Regarding the notation '$\times$' as a tensor product $\otimes$, we can map a state in the one-particle Liouville space $|\alpha,\beta\rangle\rangle$ to a state in the two-particle Hilbert space $|\alpha,\beta\rangle$, details of which are given in Sec. 3.1. Then, obtaining the Green's function of L_0 is equivalent to obtaining the Green's function of the following Hamiltonian:

$$\mathcal{H}_0 = -t\sum_{x=-\infty}^{\infty}\left(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x\right) + t\sum_{-\infty}^{\infty}\left(b_x^\dagger b_{x+1} + b_{x+1}^\dagger b_x\right), \tag{2.41}$$

where $a_x^\dagger$, a_x, $b_x^\dagger$, b_x are the creation and annihilation operators of distinguishable particles, respectively. Using the above-mentioned property, we obtain the Fourier transformation of G_0 as follows;

$$\langle\langle x_1, x_2|G_0|x_3, x_4\rangle\rangle = \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} e^{ik_1(x_1-x_3)} \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} e^{-ik_2(x_2-x_4)} \frac{1}{z + 2t\cos k_1 - 2t\cos k_2}. \tag{2.42}$$

Thus Eqs. (2.32)–(2.35) are Fourier transformed as follows:

$$\begin{aligned} G^{0d}(k;d) &= \frac{1}{z+2t\cos k} - t_1^2 \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{G^{0d}(d;k_2)}{(z+2t\cos k)(z+2t\cos k - 2t\cos k_2)} \\ &\quad + t_1^2\, G^{0d}(k;d) \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{1}{(z+2t\cos k)(z+2t\cos k - 2t\cos k_2)}, \end{aligned} \tag{2.43}$$

$$\begin{aligned} G^{0d}(d;k) &= t_1^2\, G^{0d}(d;k) \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \frac{1}{(z-2t\cos k)(z+2t\cos k_1 - 2t\cos k)} \\ &\quad - t_1^2 \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \frac{G^{0d}(k_1;d)}{(z-2t\cos k)(z+2t\cos k_1 - 2t\cos k)}, \end{aligned} \tag{2.44}$$

$$\begin{aligned} G^{d0}(d;k) &= \frac{1}{z-2t\cos k} - t_1^2 \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{G^{d0}(k_2;d)}{(z-2t\cos k)(z-2t\cos k + 2t\cos k_2)} \\ &\quad + t_1^2\, G^{d0}(d;k) \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{1}{(z-2t\cos k)(z-2t\cos k + 2t\cos k_2)}, \end{aligned} \tag{2.45}$$

$$\begin{aligned} G^{d0}(k;d) &= t_1^2\, G^{d0}(k;d) \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \frac{1}{(z+2t\cos k)(z-2t\cos k_1 + 2t\cos k)} \\ &\quad - t_1^2 \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{G^{d0}(d;k_2)}{(z+2t\cos k)(z-2t\cos k_2 + 2t\cos k)}. \end{aligned} \tag{2.46}$$

Then our original problem (2.20) reduces to the following equation:

$$z = t_1^2 \int_{-\pi}^{\pi} \frac{dk}{2\pi} (G^{0d}(k;d) + G^{d0}(d;k) - G^{0d}(d;k) - G^{d0}(k;d)). \tag{2.47}$$

The integral terms indicate the effects of entanglement of the bra state and the ket state. If the bra state and the ket state are not entangled, all the eigenvalues of the original Liouvillian should be of the type of $E_\alpha - E_\beta$. Thus eigenvalues that are not expected from the corresponding Hamiltonian should come from the integral terms.

In the next section, we calculate the eigenvalues of the Liouvillian that are not predictable from the eigenvalues of the corresponding Hamiltonian in the second order of t_1. The second-order perturbation is the lowest-order approximation for considering the effects of the integral terms, as can be seen in Eqs. (2.43)–(2.46).

2.4 Perturbation analysis of nontrivial eigenvalues

In the present section, we first obtain trivial eigenvalues of the type of $E_\alpha - E_\beta$ and then nontrivial eigenvalues by the second-order perturbation analysis of Eqs. (2.43)–(2.46). In

Sec. 2.4.1, we obtain the trivial eigenvalues by extending the domain of the integral after integrating all terms. On the other hand, in Sec. 2.4.2, we obtain the nontrivial eigenvalues by extending the domain of the integral where we integrate only terms implying the entanglement of the bra state and the ket state.

2.4.1 Trivial eigenvalues

Let us show how to obtain the trivial eigenvalues of the Liouvillian in the present subsection. We use Eqs. (2.43)–(2.46), which we introduce in Sec. 2.3, and Eq. (2.47). First, we calculate the following integral term in Eqs. (2.43)–(2.46):

$$\begin{aligned}
F^{\pm}(k) &:= \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{1}{(z \pm 2t\cos k)(z \pm 2t\cos k \mp 2t\cos k_2)} \\
&= \frac{1}{z \pm 2t\cos k} \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \frac{1}{z \pm 2t\cos k \mp 2t\cos k_2} \\
&= \frac{1}{E^{\pm}} \int_{-\infty}^{\infty} \frac{dx}{\pi} \frac{1}{(1+x^2)E^{\pm} \mp 2t(1-x^2)} \\
&= \frac{1}{E^{\pm}(E^{\pm} \pm 2t)} \int_{-\infty}^{\infty} \frac{dx}{\pi} \frac{1}{(x + \sqrt{\frac{-E^{\pm}\pm 2t}{E^{\pm}\pm 2t}})(x - \sqrt{\frac{-E^{\pm}\pm 2t}{E^{\pm}\pm 2t}})},
\end{aligned} \tag{2.48}$$

where the double sign is in the same order, $E^{\pm} = z \pm 2t\cos k$ and for all α

$$\mathrm{Re}\sqrt{\alpha} > 0. \tag{2.49}$$

In the third line of Eq. (2.48), the variable k is transformed to the variable x as $x = \tan k/2$.

For Im $z > 0$, we have the results

$$F^{+}(k) = -\frac{i}{z + 2t\cos k} \frac{1}{\sqrt{4t^2 - (z + 2t\cos k)^2}}, \tag{2.50}$$

$$F^{-}(k) = \frac{i}{z - 2t\cos k} \frac{1}{\sqrt{4t^2 - (z - 2t\cos k)^2}}, \tag{2.51}$$

because of the following relations:

$$\mathrm{Im}\sqrt{\frac{-z - 2t\cos k + 2t}{z + 2t\cos k + 2t}} < 0, \tag{2.52}$$

$$\mathrm{Im}\sqrt{\frac{-z + 2t\cos k - 2t}{z - 2t\cos k - 2t}} > 0, \tag{2.53}$$

where k is real and t is positive. For Im $z < 0$, we have

$$F^{+}(k) = \frac{i}{z + 2t\cos k} \frac{1}{\sqrt{4t^2 - (z + 2t\cos k)^2}}, \tag{2.54}$$

$$F^{-}(k) = -\frac{i}{z - 2t\cos k} \frac{1}{\sqrt{4t^2 - (z - 2t\cos k)^2}}. \tag{2.55}$$

Since it is not a simple problem to solve Eq. (2.47) generally, we concentrate on eigenvalues near $z = 0$. Suppose that the eigenvalue z is expanded as follows:

$$z = t_1^2 \xi + O(t_1^3), \tag{2.56}$$

and then

$$\xi = \lim_{t_1 \to 0} \frac{z}{t_1^2}. \tag{2.57}$$

Hereafter we consider the case Im $z < 0$. Using Eq. (2.57), we transform Eqs. (2.43)–(2.46) as follows:

$$\begin{aligned}\lim_{t_1 \to 0} t_1^2 G^{0d}(k;d) = \lim_{t_1 \to 0} \Bigg[& \frac{1}{\xi + \frac{2t}{t_1^2}\cos k} - \frac{2}{t_1^2}\int_0^\pi \frac{dk_2}{2\pi} \frac{t_1^2 G^{0d}(d;k_2)}{(\xi + \frac{2t}{t_1^2}\cos k)(\xi + \frac{2t}{t_1^2}\cos k - \frac{2t}{t_1^2}\cos k_2)} \\ & + t_1^2 G^{0d}(k;d) \frac{i}{(\xi + \frac{2t}{t_1^2}\cos k)\sqrt{4t^2 - t_1^4(\xi + \frac{2t}{t_1^2}\cos k)^2}} \Bigg],\end{aligned} \tag{2.58}$$

$$\begin{aligned}\lim_{t_1 \to 0} t_1^2 G^{0d}(d;k) = \lim_{t_1 \to 0} \Bigg[& -\frac{2}{t_1^2}\int_0^\pi \frac{dk_1}{2\pi} \frac{t_1^2 G^{0d}(k_1;d)}{(\xi - \frac{2t}{t_1^2}\cos k)(\xi - \frac{2t}{t_1^2}\cos k + \frac{2t}{t_1^2}\cos k_1)} \\ & - t_1^2 G^{0d}(d;k) \frac{i}{(\xi - \frac{2t}{t_1^2}\cos k)\sqrt{4t^2 - t_1^4(\xi - \frac{2t}{t_1^2}\cos k)^2}} \Bigg],\end{aligned} \tag{2.59}$$

$$\begin{aligned}\lim_{t_1 \to 0} t_1^2 G^{d0}(d;k) = \lim_{t_1 \to 0} \Bigg[& \frac{1}{\xi - \frac{2t}{t_1^2}\cos k} - \frac{2}{t_1^2}\int_0^\pi \frac{dk_1}{2\pi} \frac{t_1^2 G^{d0}(k_1;d)}{(\xi - \frac{2t}{t_1^2}\cos k)(\xi - \frac{2t}{t_1^2}\cos k + \frac{2t}{t_1^2}\cos k_2)} \\ & - t_1^2 G^{d0}(d;k) \frac{i}{(\xi - \frac{2t}{t_1^2}\cos k)\sqrt{4t^2 - t_1^4(\xi - \frac{2t}{t_1^2}\cos k)^2}} \Bigg],\end{aligned} \tag{2.60}$$

$$\begin{aligned}\lim_{t_1 \to 0} t_1^2 G^{d0}(k;d) = \lim_{t_1 \to 0} \Bigg[& -\frac{2}{t_1^2}\int_0^\pi \frac{dk_1}{2\pi} \frac{t_1^2 G^{d0}(d;k_1)}{(\xi + \frac{2t}{t_1^2}\cos k)(\xi + \frac{2t}{t_1^2}\cos k - \frac{2t}{t_1^2}\cos k_1)} \\ & + t_1^2 G^{d0}(k;d) \frac{i}{(\xi + \frac{2t}{t_1^2}\cos k)\sqrt{4t^2 - t_1^4(\xi + \frac{2t}{t_1^2}\cos k)^2}} \Bigg],\end{aligned} \tag{2.61}$$

where we used the fact that the Green's functions such as $G^{0d}(k;d)$ are even functions with respect to k, as we have seen in Eqs. (2.43)–(2.46). By transforming the variable as $q = (2t/t_1^2)\cos k_1$, we have the integral measure as follows:

$$\frac{2}{t_1^2}\int_0^\pi \frac{dk_1}{2\pi} = \frac{1}{t}\int_{-2t/t_1^2}^{2t/t_1^2} \frac{dq}{2\pi} \frac{1}{\sqrt{1 - (t_1^2/2t)^2 q^2}}. \tag{2.62}$$

If $f(q)$ is a function that decays faster than $1/q^2$, the integral term is given in the following form:

$$\lim_{t_1\to 0}\frac{1}{t}\int_{-2t/t_1^2}^{2t/t_1^2}\frac{dq}{2\pi}\frac{f(q)}{\sqrt{1-(t_1^2/2t)^2q^2}}=\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq}{2\pi}f(q). \tag{2.63}$$

Using the new Green's functions defined as

$$\mathcal{G}^{0d}(q;d):=\lim_{t_1\to 0}t_1^2\,G^{0d}(k;d), \tag{2.64}$$

$$\mathcal{G}^{0d}(d;q):=\lim_{t_1\to 0}t_1^2\,G^{0d}(d;k), \tag{2.65}$$

$$\mathcal{G}^{d0}(d;q):=\lim_{t_1\to 0}t_1^2\,G^{d0}(d;k), \tag{2.66}$$

$$\mathcal{G}^{d0}(q;d):=\lim_{t_1\to 0}t_1^2\,G^{d0}(k;d), \tag{2.67}$$

and Eq. (2.63), we can simplify Eqs. (2.58)–(2.61) as follows:

$$\mathcal{G}^{0d}(q;d)=\frac{1}{\xi+q}-\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{0d}(d;q_2)}{(\xi+q)(\xi+q-q_2)}+\frac{i}{2t}\frac{\mathcal{G}^{0d}(q;d)}{(\xi+q)}, \tag{2.68}$$

$$\mathcal{G}^{0d}(d;q)=-\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{(\xi-q)(\xi-q+q_1)}-\frac{i}{2t}\frac{\mathcal{G}^{0d}(d;q)}{(\xi-q)}, \tag{2.69}$$

$$\mathcal{G}^{d0}(d;q)=\frac{1}{\xi-q}-\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(q_2;d)}{(\xi-q)(\xi-q+q_2)}-\frac{i}{2t}\frac{\mathcal{G}^{d0}(d;q)}{(\xi-q)}, \tag{2.70}$$

$$\mathcal{G}^{d0}(q;d)=-\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{d0}(d;q_1)}{(\xi+q)(\xi+q-q_1)}+\frac{i}{2t}\frac{\mathcal{G}^{d0}(q;d)}{(\xi+q)}. \tag{2.71}$$

Thus in the case of Im $\xi<0$, the equations to be solved are as follows:

$$\xi=\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq}{2\pi}(\mathcal{G}^{0d}(q;d)+\mathcal{G}^{d0}(d;q)-\mathcal{G}^{0d}(d;q)-\mathcal{G}^{d0}(q;d)), \tag{2.72}$$

$$\mathcal{G}^{0d}(q;d)=\frac{1}{q+\xi-\frac{i}{2t}}+\frac{1}{q+\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{0d}(d;q_2)}{q_2-q-\xi}, \tag{2.73}$$

$$\mathcal{G}^{0d}(d;q)=\frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{q_1-q+\xi}, \tag{2.74}$$

$$\mathcal{G}^{d0}(d;q)=-\frac{1}{q-\xi-\frac{i}{2t}}+\frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(q_2;d)}{(q_2-q+\xi)}, \tag{2.75}$$

$$\mathcal{G}^{d0}(q;d)=\frac{1}{q+\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(d;q_2)}{q_2-q-\xi}. \tag{2.76}$$

Let us solve Eq. (2.72) for Im $\xi<0$. First, substituting Eq. (2.74) into Eq. (2.73), we obtain the closed equation

$$\begin{aligned}\mathcal{G}^{0d}(q;d)=&\frac{1}{q+\xi-\frac{i}{2t}}\\&-\frac{1}{q+\xi-\frac{i}{2t}}\frac{1}{t^2}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{(q_2-q-\xi)(q_2-\xi-\frac{i}{2t})(q_2-q_1-\xi)}.\end{aligned} \tag{2.77}$$

1. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) < 0$:

   Regarding the integrand as a function of q_2, we find that the poles are all in the lower half plane. By closing the contour of q_2 in the upper half plane, we can eliminate the integral. Therefore, Eq. (2.77) reduces to

$$\mathcal{G}^{0d}(q;d) = \frac{1}{q+\xi-\frac{i}{2t}}. \tag{2.78}$$

2. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) > 0$:

   Regarding the integrand as a function of q_2, we find that the poles $q+\xi$ and $q_1+\xi$ are in the lower half plane and the other pole $\xi + i/(2t)$ is in the upper half plane. The integration with respect to q_2 then gives

$$\begin{aligned}\mathcal{G}^{0d}(q;d) &= \frac{1}{q+\xi-\frac{i}{2t}} - \frac{1}{q+\xi-\frac{i}{2t}}\frac{i}{t^2}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{(q-\frac{i}{2t})(q_1-\frac{i}{2t})} \\ &= \frac{1}{q+\xi-\frac{i}{2t}},\end{aligned} \tag{2.79}$$

   where we used in the second equation the fact that $\mathcal{G}^{0d}(q;d)$ has only the poles $-\xi + i/(2t)$ and $i/(2t)$ in the upper half plane.

Substituting the above results into Eq. (2.74), we obtain

$$\begin{aligned}\mathcal{G}^{0d}(d;q) &= \frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{1}{(q_1-q+\xi)(q_1+\xi-\frac{i}{2t})} \\ &= 0,\end{aligned} \tag{2.80}$$

because both poles $q-\xi$ and $-\xi+\frac{i}{2t}$ are in the upper half plane.

Next, substituting Eq. (2.76) into Eq. (2.75), we obtain the closed equation

$$\begin{aligned}\mathcal{G}^{d0}(d;q) = &-\frac{1}{q-\xi-\frac{i}{2t}} \\ &-\frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t^2}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{d0}(d;q_1)}{(q_2-q+\xi)(q_2+\xi-\frac{i}{2t})(q_2-q_1+\xi)}.\end{aligned} \tag{2.81}$$

Regarding the integrand as a function of q_2, we find that all the poles $q-\xi$, $-\xi+i/(2t)$ and $q_1-\xi$ are in the upper half plane. Then Eq. (2.81) reduces to

$$\mathcal{G}^{d0}(d;q) = -\frac{1}{q-\xi-\frac{i}{2t}}. \tag{2.82}$$

Substituting Eq. (2.82) into Eq. (2.76), we obtain

$$\mathcal{G}^{d0}(q;d) = -\frac{1}{q+\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{1}{(q_2-q-\xi)(q_2-\xi-\frac{i}{2t})}. \tag{2.83}$$

1. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) < 0$:

   The poles of the integrand of (2.83) are both in the lower half plane. Therefore, we have

$$\mathcal{G}^{d0}(q; d) = 0. \tag{2.84}$$

2. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) > 0$:

   The pole $q+\xi$ is in the lower half plane, and the other pole $\xi + i/(2t)$ is in the upper half plane. Then the residue integral gives

$$\mathcal{G}^{d0}(q; d) = \frac{i}{t} \frac{1}{(q + \xi - \frac{i}{2t})(q - \frac{i}{2t})}. \tag{2.85}$$

By substituting the above results into Eq. (2.72), we obtain the following equations to be solved in the case of $\mathrm{Im}\ \xi < 0$.

1. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) < 0$:

$$\begin{aligned} \xi &= \frac{1}{t} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \left(\frac{1}{q + \xi - \frac{i}{2t}} - \frac{1}{q - \xi - \frac{i}{2t}} \right) \\ &= \frac{1}{t} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{-2\xi}{(q + \xi - \frac{i}{2t})(q - \xi - \frac{i}{2\pi})} \\ &= \frac{i}{t}. \end{aligned} \tag{2.86}$$

2. The case of $\mathrm{Im}(\xi + \mathrm{i}/(2t)) > 0$:

$$\begin{aligned} \xi &= \frac{1}{t} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \left[\frac{1}{q + \xi - \frac{i}{2t}} - \frac{1}{q - \xi - \frac{i}{2t}} - \frac{i}{t(q + \xi - \frac{i}{2t})(q - \frac{i}{2t})} \right] \\ &= 0. \end{aligned} \tag{2.87}$$

In both cases, the solutions do not meet the condition $\mathrm{Im}\ z < 0$. However, as we can see in Appendix A.1, the complex eigenvalues of the Hamiltonian are also improper solutions; the complex eigenvalues of the Hamiltonian are the poles of the Green's function in an expanded domain by analytic continuation (see Fig. 2.3). Because of the dispersion relation of the present particle $E = -2t \cos k$, the energy has two Riemann sheets in its complex plane. Since the resonant solutions are in the second Riemann sheet, the analytic continuation must be done in the following way; when we are interested in a resonant solution in the region $\mathrm{Im}\ E < 0$, we must proceed from the region $\mathrm{Im}\ E > 0$ in the first Riemann sheet. Therefore, it is reasonable to set $\mathrm{Im}\ E > 0$ in the zeroth-order perturbation in order to find a resonant solution in the region $\mathrm{Im}\ E < 0$. Then the above two solutions (2.86) and (2.87) may also have physical meaning.

According to Appendix A.1, the eigenvalues of the corresponding Hamiltonian are the following:

$$E = \pm \sqrt{2t^2 + \sqrt{4t^4 + t_1^4}}, \tag{2.88}$$

$$E = \pm i \sqrt{\sqrt{4t^4 + t_1^4} - 2t^2}. \tag{2.89}$$

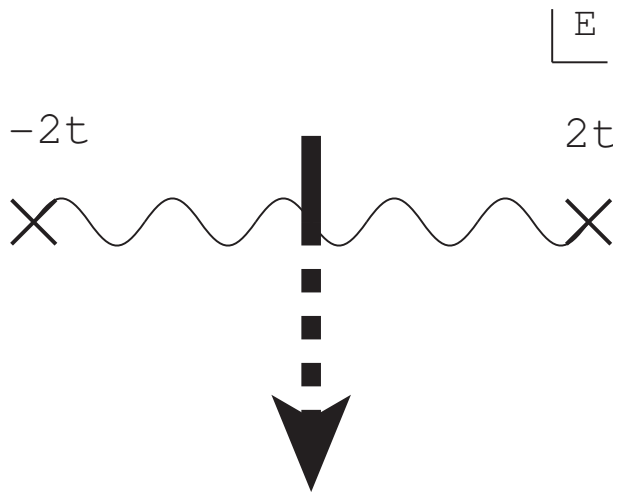

Figure 2.3: The basic concept for the analytic continuation

Thus the trivial eigenvalues $E_\alpha - E_\beta$ near $z = 0$ should be the following:

$$z = \pm\frac{i}{t}t_1^2 + O(t_1^3), \tag{2.90}$$

$$z = 0. \tag{2.91}$$

Then the solutions (2.86) and (2.87) can be understood as trivial eigenvalues of the Liouvillian.

In the case of Im $\xi > 0$, instead of Eqs. (2.72)–(2.76), the equations to be solved are now the following:

$$\xi = \frac{1}{t}\int_{-\infty}^{\infty}\frac{dq}{2\pi}(\mathcal{G}^{0d}(q;d) + \mathcal{G}^{d0}(d;q) - \mathcal{G}^{0d}(d;q) - \mathcal{G}^{d0}(q;d)), \tag{2.92}$$

$$\mathcal{G}^{0d}(q;d) = \frac{1}{q+\xi+\frac{i}{2t}} + \frac{1}{q+\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{0d}(d;q_2)}{q_2-q-\xi}, \tag{2.93}$$

$$\mathcal{G}^{0d}(d;q) = \frac{1}{q-\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{q_1-q+\xi}, \tag{2.94}$$

$$\mathcal{G}^{d0}(d;q) = -\frac{1}{q-\xi+\frac{i}{2t}} + \frac{1}{q-\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(q_2;d)}{q_2-q+\xi}, \tag{2.95}$$

$$\mathcal{G}^{d0}(q;d) = \frac{1}{q+\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(d;q_2)}{q_2-q-\xi}. \tag{2.96}$$

In the same way as in the case of Im $\xi < 0$, we obtain the eigenvalues of the Liouvillian in the case of Im $\xi > 0$;

1. The case of $\mathrm{Im}(\xi - \frac{i}{2t}) > 0$:

$$\xi = -\frac{i}{t}, \tag{2.97}$$

2. The case of $\mathrm{Im}(\xi - \frac{i}{2t}) < 0$:

$$\xi = 0. \tag{2.98}$$

These are other trivial eigenvalues near $z = 0$.

2.4.2 Nontrivial eigenvalues

In what follows, we show the nontrivial eigenvalues though it is not clear for the moment whether these have physical meaning or not. The way to obtain the eigenvalues are somewhat arbitrary. Since we have not reached clear understanding of boundary conditions that are necessary to obtain the nontrivial and physically relevant eigenvalues of the Liouvillian, we try to obtain the eigenvalues in various ways.

First, we consider the case $\mathrm{Im}\ \xi < 0$. We nonetheless use the following functions:

$$F^+(k) = -\frac{i}{z + 2t\cos k}\frac{1}{\sqrt{4t^2 - (z + 2t\cos k)^2}}, \tag{2.99}$$

$$F^-(k) = -\frac{i}{z - 2t\cos k}\frac{1}{\sqrt{4t^2 - (z - 2t\cos k)^2}}. \tag{2.100}$$

Here $F^-(k)$ is the original function for $\mathrm{Im}\ z < 0$ as in Eq. (2.54) but $F^+(k)$ is redefined by the analytic continuation. In this case, the equations to be solved are the following:

$$\xi = \frac{1}{t}\int_{-\infty}^{\infty}\frac{dq}{2\pi}(\mathcal{G}^{0d}(q;d) + \mathcal{G}^{d0}(d;q) - \mathcal{G}^{0d}(d;q) - \mathcal{G}^{d0}(q;d)) \tag{2.101}$$

$$\mathcal{G}^{0d}(q;d) = \frac{1}{q+\xi+\frac{i}{2t}} + \frac{1}{q+\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{0d}(d;q_2)}{q_2 - q - \xi}, \tag{2.102}$$

$$\mathcal{G}^{0d}(d;q) = \frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{q_1 - q + \xi}, \tag{2.103}$$

$$\mathcal{G}^{d0}(d;q) = -\frac{1}{q-\xi-\frac{i}{2t}} + \frac{1}{q-\xi-\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(q_2;d)}{q_2 - q + \xi}, \tag{2.104}$$

$$\mathcal{G}^{d0}(q;d) = \frac{1}{q+\xi+\frac{i}{2t}}\frac{1}{t}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\frac{\mathcal{G}^{d0}(d;q_2)}{q_2 - q - \xi}. \tag{2.105}$$

First in the case of $\mathrm{Im}\ \xi < 0$ and $\mathrm{Im}(\xi + i/(2t)) < 0$, any appropriate solutions do not exist. Next, we consider the case of $\mathrm{Im}\ \xi < 0$ and $\mathrm{Im}(\xi + i/(2t)) > 0$. Substituting Eq. (2.103) into Eq. (2.102) and integrating the second term, we obtain the closed equation

$$\begin{aligned}\mathcal{G}^{0d}(q;d) &= \frac{1}{q+\xi+\frac{i}{2t}} \\ &+ \frac{1}{q+\xi+\frac{i}{2t}}\frac{1}{t^2}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{(q_2-q-\xi)(q_2-\xi-\frac{i}{2t})(q_1-q_2+\xi)} \\ &= \frac{1}{q+\xi+\frac{i}{2t}} - \frac{1}{(q+\xi+\frac{i}{2t})(q-\frac{i}{2t})}\frac{i}{t^2}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\frac{\mathcal{G}^{0d}(q_1;d)}{q_1-\frac{i}{2t}}.\end{aligned} \tag{2.106}$$

As we can see in the above equation, the pole of the Green's function in the lower half plane is only $-\xi - i/(2t)$. Let us define α as follows:

$$\alpha := \lim_{q \to -\xi - \frac{i}{2t}} \left(q + \xi + \frac{i}{2t} \right) \mathcal{G}^{0d}(q; d). \tag{2.107}$$

Then we obtain the following equation:

$$\mathcal{G}^{0d}(q; d) = \frac{1}{q + \xi + \frac{i}{2t}} - \frac{1}{t^2} \frac{\alpha}{(q + \xi + \frac{i}{2t})(q - \frac{i}{2t})(-\xi - \frac{i}{t})}. \tag{2.108}$$

By applying $\lim_{q \to -\xi - i/(2t)}(q + \xi + i/(2t))$ on the both sides of Eq. (2.108), we have

$$\alpha = 1 - \frac{1}{t^2} \frac{\alpha}{(-\xi - \frac{i}{t})(-\xi - \frac{i}{t})}, \tag{2.109}$$

which is followed by

$$\alpha = \frac{(t\xi + i)^2}{1 + (t\xi + i)^2}. \tag{2.110}$$

Substituting Eq. (2.110) into Eq. (2.108), we arrive at

$$\mathcal{G}^{0d}(q; d) = \frac{1}{q + \xi + \frac{i}{2t}} + \frac{\xi + \frac{i}{t}}{(q + \xi + \frac{i}{2t})(q - \frac{i}{2t})[(t\xi + i)^2 + 1]}. \tag{2.111}$$

Using this result, we similarly obtain the other Green's functions as follows:

$$\mathcal{G}^{0d}(d; q) = \frac{i}{t(q - \xi - \frac{i}{2t})(q + \frac{i}{2t})} \left[1 - \frac{1}{(t\xi + i)^2 + 1} \right], \tag{2.112}$$

$$\mathcal{G}^{d0}(d; q) = -\frac{1}{q - \xi - \frac{i}{2t}} + \frac{\xi + \frac{i}{t}}{(q - \xi - \frac{i}{2t})(q + \frac{i}{2t})[(t\xi + i)^2 + 1]}, \tag{2.113}$$

$$\mathcal{G}^{d0}(q; d) = \frac{i}{t(q + \xi + \frac{i}{2t})(q - \frac{i}{2t})} \left[1 - \frac{1}{(t\xi + i)^2 + 1} \right]. \tag{2.114}$$

Substituting the above functions into Eq. (2.101), we obtain the equation as follows:

$$\xi = -\frac{i}{t} + \frac{i}{t} \frac{2}{(t\xi + i)^2 + 1} + \frac{2}{t(t\xi + i)} - \frac{2}{t(t\xi + i)\left[(t\xi + i)^2 + 1\right]}. \tag{2.115}$$

The equation is written in terms of $ix = t\xi + i$ as

$$x(x + 1)(x^2 - x + 2) = 0, \tag{2.116}$$

which is solved as

$$t\xi = \frac{z}{t_1^2} t = -i, \quad -2i, \quad -\frac{i}{2} \pm \frac{\sqrt{7}}{2}. \tag{2.117}$$

Since we consider the case of Im $\xi < 0$ and $\mathrm{Im}(\xi + i/(2t)) > 0$, the appropriate solution is only $t\xi = -i/2 \pm \sqrt{7}/2$, which is a nontrivial eigenvalue. (The solution is actually on the line $\mathrm{Im}(\xi + i/(2t)) = 0$, which puts the pole on the real axis. We can avoid the pole by shifting the pole infinitesimally.)

Next, we consider the case of Im $z > 0$. We now use

$$F^+(k) = \frac{i}{z + 2t\cos k} \frac{1}{\sqrt{4t^2 - (z + 2t\cos k)^2}}, \tag{2.118}$$

$$F^-(k) = \frac{i}{z - 2t\cos k} \frac{1}{\sqrt{4t^2 - (z - 2t\cos k)^2}}. \tag{2.119}$$

We obtain the solution $t\xi = i/2 \pm \sqrt{7}/2$ in the same way.

We thus obtained the trivial eigenvalues of the Liouvillian by expanding the domain of the integral after we integrate all the terms. On the other hand, we obtained the nontrivial eigenvalues by expanding the domain of $F^+(k)$ or $F^-(k)$ by analytic continuation. As in the discussion of Appendix A.1, the above nontrivial 'eigenvalues' are not the eigenvalues in the proper sense of the word. In the future works, we should clarify what physical meaning, if any, these nontrivial eigenvalues have.

Chapter 3

The method of rigorous solution

3.1 Correspondence between one-particle Liouvillian and two-particle Hamiltonian

Let us introduce the method of obtaining the rigorous solution of the eigenvalue problem of the Liouvillian in this section. We show that the one-particle Green's function of QLQ is equal to the two-particle Green's function of a new Hamiltonian $\mathcal{H}$. In order to map the eigenvalue problem of the Liouvillian to the eigenvalue problem of the Hamiltonian, we use some powerful methods; i.e. the Dyson equation, closure, and so on.

In this section, the models are as follows (Fig. 3.1):

$$H = -t\sum_{-\infty}^{\infty}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) - t_1(c_{d0}^\dagger c_0 + c_0^\dagger c_{d0}) + \sum_{i,j} v_{ij}(c_{di}^\dagger c_{dj} + c_{dj}^\dagger c_{di}), \tag{3.1}$$

where c_x, c_{di}, $c_x^\dagger$, $c_{di}^\dagger$ are the annihilation and creation operators at the site x and d_i, respectively. Using the operation '$\times$' defined in Appendix A.3, we obtain QLQ as follows:

$$\begin{aligned} QLQ =& Q_{\mathrm{s}}HQ_{\mathrm{s}} \times I_{\mathrm{s}} - I_{\mathrm{s}} \times Q_{\mathrm{s}}HQ_{\mathrm{s}} \\ &+ Q_{\mathrm{s}}HP_{\mathrm{s}} \times Q_{\mathrm{s}} - Q_{\mathrm{s}} \times P_{\mathrm{s}}HQ_{\mathrm{s}} \\ &+ P_{\mathrm{s}}HQ_{\mathrm{s}} \times Q_{\mathrm{s}} - Q_{\mathrm{s}} \times Q_{\mathrm{s}}HP_{\mathrm{s}} \\ &+ P_{\mathrm{s}}HP_{\mathrm{s}} \times Q_{\mathrm{s}} - Q_{\mathrm{s}} \times P_{\mathrm{s}}HP_{\mathrm{s}}. \end{aligned} \tag{3.2}$$

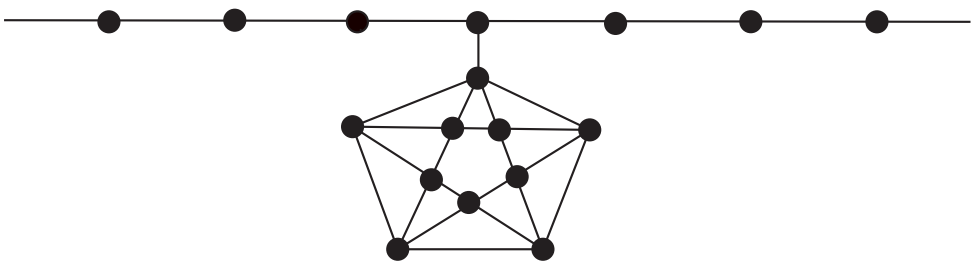

Figure 3.1: T-type quantum dot model. The number of the sites in the dot is N.

In this case, PLP does not vanish and $L_{\rm eff}$ in Eq. (2.15) is an $N^2 \times N^2$ matrix, where N is the number of the sites on the dot. Thus we need the following matrix elements:

$$\begin{aligned}\langle\langle d_i, d_j|L_{\rm eff}|d_{i'}, d_{j'}\rangle\rangle &= \langle\langle d_i, d_j|PLP|d_{i'}, d_{j'}\rangle\rangle \\ &+ t_1^2\left(\delta_{i,0}\delta_{i',0}\langle\langle 0, d_j|\frac{1}{z-QLQ}|0, d_j\rangle\rangle - \delta_{i,0}\delta_{j',0}\langle\langle 0, d_j|\frac{1}{z-QLQ}|d_{i'}, 0\rangle\rangle\right. \\ &\left.-\delta_{i',0}\delta_{j,0}\langle\langle d_i, 0|\frac{1}{z-QLQ}|0, d_{j'}\rangle\rangle + \delta_{j,0}\delta_{j',0}\langle\langle d_i, 0|\frac{1}{z-QLQ}|d_{i'}, 0\rangle\rangle\right).\end{aligned} \tag{3.3}$$

We need to obtain the Green's function of QLQ for solving the original eigenvalue problem of the Liouvillian.

Though QLQ is a super-operator which acts on density operators, the density operators belong to a Hilbert space with the inner product (A.41) in Appendix A.3. Therefore, we can treat QLQ as a usual operator which acts on the Hilbert space spanned by the states $|i, j\rangle\rangle$.

Let us here introduce a two-particle Hamiltonian:

$$\begin{aligned}\mathcal{H} &= -t\sum_{x=-\infty}^{\infty}(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x) + t\sum_{-\infty}^{\infty}(b_x^\dagger b_{x+1} + b_x^\dagger b_x) \\ &- t_1(a_0^\dagger d_0^a + d_0^{a\dagger} a_0)\left(1 - \sum_i d_i^{b\dagger} d_i^b\right) + t_1\left(1 - \sum_i d_i^{a\dagger} d_i^a\right)(b_0^\dagger d_0^b + d_0^{b\dagger} b_0) \\ &+ \left[\sum_{i,j} v_{ij}(d_i^{a\dagger} d_j^a + d_j^{a\dagger} d_i^a)\right]\left(1 - \sum_{i'} d_{i'}^{b\dagger} d_{i'}^b\right) - \left(1 - \sum_{i'} d_{i'}^{a\dagger} d_{i'}^a\right)\left[\sum_{i,j} v_{ij}(d_i^{b\dagger} d_j^b + d_j^{b\dagger} d_i^b)\right],\end{aligned} \tag{3.4}$$

where $a_x^\dagger$, a_x, $b_x^\dagger$, b_x are the creation and annihilation operators of distinguishable particles at the site x on the lead, respectively, and $d_i^{a\dagger}$, d_i^a, $d_i^{b\dagger}$, d_i^b are those at the site d_i on the dot. Then the algebraic structure of $\mathcal{H}$ is exactly the same as that of QLQ in Eq. (3.2):

$$\begin{aligned}Q_{\rm s}HQ_{\rm s} \times I_{\rm s} &\longleftrightarrow -t\sum_{x=-\infty}^{\infty}(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x), \\ -I_{\rm s} \times Q_{\rm s}HQ_{\rm s} &\longleftrightarrow t\sum_{-\infty}^{\infty}(b_x^\dagger b_{x+1} + b_x^\dagger b_x), \\ Q_{\rm s}HP_{\rm s} \times Q_{\rm s} &\longleftrightarrow -t_1 a_0^\dagger d_0^a\left(1 - \sum_i d_i^{b\dagger} d_i^b\right), \\ -Q_{\rm s} \times P_{\rm s}HQ_{\rm s} &\longleftrightarrow t_1\left(1 - \sum_i d_i^{a\dagger} d_i^a\right) d_0^{b\dagger} b_0,\end{aligned} \tag{3.5}$$

$$
\begin{aligned}
P_{\rm s}HQ_{\rm s}\times Q_{\rm s} &\longleftrightarrow -t_1 d_0^{a\dagger}a_0(1-\sum_i d_i^{b\dagger}d_i),\\
-Q_{\rm s}\times Q_{\rm s}HP_{\rm s} &\longleftrightarrow t_1(1-\sum_i d_i^{a\dagger}d_i^a)b_0^\dagger d_0^b,\\
P_{\rm s}HP_{\rm s}\times Q_{\rm s} &\longleftrightarrow \left[\sum_{i,j} v_{ij}(d_i^{a\dagger}d_j^a+d_j^{a\dagger}d_i^b)\right]\left(1-\sum_i d_i^{b\dagger}d_i^b\right),\\
-Q_{\rm s}\times P_{\rm s}HP_{\rm s} &\longleftrightarrow -\left(1-\sum_i d_i^{a\dagger}d_i\right)\left[\sum_{i,j} v_{ij}(d_i^{b\dagger}d_j^b+d_j^{b\dagger}d_i^b)\right].
\end{aligned}
\tag{3.6}
$$

In this way, the original problem of obtaining the Green's function of QLQ reduces to obtaining the Green's function of the two-particle Hamiltonian $\mathcal{H}$.

We stress here that $\mathcal{H}$ has a two-body interaction such as the term $t_1 a_0^\dagger d_0^a d_i^{b\dagger} d_i^b$. This means that the evolution of the bra and ket states may correlate in the Liouville space and suggests that some of the eigenvectors are not of the form $|\alpha\rangle\langle\beta|$ and their eigenvalues z are not of the type of $E_\alpha - E_\beta$.

3.2 In the case of $N = 1$

Let us show the simple example of the previous section. We now use the same model as in the previous chapter (Fig. 2.1):

$$
H = -t\sum_{x=-\infty}^{\infty}(c_{x+1}^\dagger c_x + c_x^\dagger c_{x+1}) + (-t_1)(d^\dagger c_0 + c_0^\dagger d), \tag{3.7}
$$

where $c_x^\dagger$ and c_x are the creation and annihilation operators at the site x on the lead, respectively, while $d^\dagger$ and d are those at the dot site.

As we see in the previous chapter, the first step to solve the eigenvalue problem of the Liouvillian is obtaining the Green's function of QLQ:

$$
\begin{aligned}
QLQ = {} & Q_{\rm s}HQ_{\rm s}\times I_{\rm s} + P_{\rm s}HQ_{\rm s}\times Q_{\rm s} + Q_{\rm s}HP_{\rm s}\times Q_{\rm s}\\
& - I_{\rm s}\times Q_{\rm s}HQ_{\rm s} - Q_{\rm s}\times Q_{\rm s}HP_{\rm s} - Q_{\rm s}\times P_{\rm s}HQ_{\rm s}.
\end{aligned}
\tag{3.8}
$$

In this case of (3.7), the two-particle Hamiltonian $\mathcal{H}$ introduced in the previous section reduces to

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \mathcal{H}_0^a + \mathcal{H}_0^b + \mathcal{H}_1, \tag{3.9}
$$

$$
\begin{aligned}
\mathcal{H}_0^a &= -t\sum_{x=-\infty}^{\infty}(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x)\\
&\quad -t_1(a_d^\dagger a_0 + a_0^\dagger a_d),
\end{aligned}
\tag{3.10}
$$

$$
\begin{aligned}
\mathcal{H}_0^b &= +t\sum_{x=-\infty}^{\infty}(b_x^\dagger b_{x+1} + b_{x+1}^\dagger b_x)\\
&\quad +t_1(b_d^\dagger b_0 + b_0^\dagger b_d),
\end{aligned}
\tag{3.11}
$$

$$
\begin{aligned}
\mathcal{H}_1 &= t_1(a_0^\dagger a_d + a_d^\dagger a_0)b_{d\dagger}b_d\\
&\quad -t_1(b_0^\dagger b_d + b_d^\dagger b_0)a_d^\dagger a_d,
\end{aligned}
\tag{3.12}
$$

where the particles a and b are distinguishable and have inverted dispersion relations. In addition, we use a state vector such as

$$|\alpha, \beta\rangle = a_\alpha^\dagger b_\beta^\dagger |\text{vac}\rangle. \tag{3.13}$$

Regarding $\mathcal{H}_1$ as the perturbation term, we obtain the Green's function of $\mathcal{H}$ using the Dyson equation:

$$\frac{1}{z-\mathcal{H}} = \frac{1}{z-\mathcal{H}_0} + \frac{1}{z-\mathcal{H}_0}\mathcal{H}_1\frac{1}{z-\mathcal{H}}. \tag{3.14}$$

We need the elements where both in the initial and final states, the particle a is in the dot and the particle b is in the site $x=0$ or the particle a is in the site $x=0$ and the particle b is in the dot. To obtain such states we need the element where the final state is $\alpha = \mathrm{d}$ and $\beta = \mathrm{d}$ and the initial state is $\alpha = 0$ and $\beta = \mathrm{d}$ or $\alpha = 0$ and $\beta = \mathrm{d}$:

$$\begin{aligned}
\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle &= \langle d,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle \\
&+ \langle d,d|\frac{1}{E-\mathcal{H}_0}\mathcal{H}_1\left(|0,d\rangle\langle 0,d| + |d,0\rangle\langle d,0| + |d,d\rangle\langle d,d|\right)\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&= \langle d,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle \\
&+ \langle d,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle d,d|\mathcal{H}_1|0,d\rangle\langle 0,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ \langle d,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle d,d|\mathcal{H}_1|d,0\rangle\langle d,0|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ \langle d,d|\frac{1}{E-\mathcal{H}_0}|d,0\rangle\langle d,0|\mathcal{H}_1|d,d\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ \langle d,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle\langle 0,d|\mathcal{H}_1|d,d\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&= \langle d,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle \\
&+ t_1\langle d,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle 0,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle d,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle d,0|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle d,d|\frac{1}{E-\mathcal{H}_0}|d,0\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ t_1\langle d,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle,
\end{aligned} \tag{3.15}$$

$$
\begin{aligned}
\langle 0,d|\frac{1}{E-\mathcal{H}}|0,d\rangle &= \langle 0,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle \\
&+ t_1\langle 0,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle 0,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle 0,d|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle d,0|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle 0,d|\frac{1}{E-\mathcal{H}_0}|d,0\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ t_1\langle 0,d|\frac{1}{E-\mathcal{H}_0}|0,d\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle,
\end{aligned} \tag{3.16}
$$

$$
\begin{aligned}
\langle d,0|\frac{1}{E-\mathcal{H}}|0,d\rangle &= \langle d,0|\frac{1}{E-\mathcal{H}_0}|0,d\rangle \\
&+ t_1\langle d,0|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle 0,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle d,0|\frac{1}{E-\mathcal{H}_0}|d,d\rangle\langle d,0|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&- t_1\langle d,0|\frac{1}{E-\mathcal{H}_0}|d,0\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle \\
&+ t_1\langle d,0|\frac{1}{E-\mathcal{H}_0}|0,d\rangle\langle d,d|\frac{1}{E-\mathcal{H}}|0,d\rangle,
\end{aligned} \tag{3.17}
$$

where we used

$$
\begin{aligned}
\langle d,d|\mathcal{H}_1|0,d\rangle &= t_1 \\
\langle d,d|\mathcal{H}_1|d,0\rangle &= -t_1 \\
\langle d,0|\mathcal{H}_1|d,d\rangle &= -t_1 \\
\langle 0,d|\mathcal{H}_1|d,d\rangle &= t_1.
\end{aligned}
$$

Let us define new notations:

$$
\mathcal{G}_{\alpha\beta;\alpha'\beta'} = \langle \alpha,\beta|\frac{1}{z-\mathcal{H}}|\alpha',\beta'\rangle, \tag{3.18}
$$

$$
\mathcal{G}^{(0)}_{\alpha\beta;\alpha'\beta'} = \langle \alpha,\beta|\frac{1}{z-\mathcal{H}_0}|\alpha',\beta'\rangle, \tag{3.19}
$$

$$
(\alpha,\alpha' = 0,d, \quad \beta,\beta' = 0,d).
$$

Then Eqs. (3.15)–(3.17) and the other equations that we need are summarized as follows:

$$
\begin{pmatrix} \mathcal{G}_{0d;0d} \\ \mathcal{G}_{d0;0d} \\ \mathcal{G}_{dd;0d} \end{pmatrix} = \begin{pmatrix} \mathcal{G}^{(0)}_{0d;0d} \\ \mathcal{G}^{(0)}_{d0;0d} \\ \mathcal{G}^{(0)}_{dd;0d} \end{pmatrix} + t_1 \begin{pmatrix} \mathcal{G}^{(0)}_{0d;dd} & -\mathcal{G}^{(0)}_{0d;dd} & \mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{0d;d0} \\ \mathcal{G}^{(0)}_{d0;dd} & -\mathcal{G}^{(0)}_{d0;dd} & \mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{d0;d0} \\ \mathcal{G}^{(0)}_{dd;dd} & -\mathcal{G}^{(0)}_{dd;dd} & \mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{dd;d0} \end{pmatrix} \begin{pmatrix} \mathcal{G}_{0d;0d} \\ \mathcal{G}_{d0;0d} \\ \mathcal{G}_{dd;0d} \end{pmatrix}, \tag{3.20}
$$

$$
\begin{pmatrix} \mathcal{G}_{0d;d0} \\ \mathcal{G}_{d0;d0} \\ \mathcal{G}_{dd;d0} \end{pmatrix} = \begin{pmatrix} \mathcal{G}^{(0)}_{0d;d0} \\ \mathcal{G}^{(0)}_{d0;d0} \\ \mathcal{G}^{(0)}_{dd;d0} \end{pmatrix} + t_1 \begin{pmatrix} \mathcal{G}^{(0)}_{0d;dd} & -\mathcal{G}^{(0)}_{0d;dd} & \mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{0d;d0} \\ \mathcal{G}^{(0)}_{d0;dd} & -\mathcal{G}^{(0)}_{d0;dd} & \mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{d0;d0} \\ \mathcal{G}^{(0)}_{dd;dd} & -\mathcal{G}^{(0)}_{dd;dd} & \mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{dd;d0} \end{pmatrix} \begin{pmatrix} \mathcal{G}_{0d;d0} \\ \mathcal{G}_{d0;d0} \\ \mathcal{G}_{dd;d0} \end{pmatrix}. \tag{3.21}
$$

Solving the above equations, we obtain

$$\begin{pmatrix}\mathcal{G}_{0d;0d}\\ \mathcal{G}_{d0;0d}\\ \mathcal{G}_{dd;0d}\end{pmatrix} = \frac{1}{D}\begin{pmatrix} \mathcal{G}^{(0)}_{0d;0d} + t_1\left[\left(\mathcal{G}^{(0)}_{d0;dd}+\mathcal{G}^{(0)}_{dd;d0}\right)\mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{0d;d0}\mathcal{G}^{(0)}_{dd;0d}\right] \\ \quad +{t_1}^2\left[\left(\mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{dd;d0} - \mathcal{G}^{(0)}_{d0;d0}\mathcal{G}^{(0)}_{dd;dd}\right)\mathcal{G}^{(0)}_{0d;0d} \right.\\ \quad\quad + \left(\mathcal{G}^{(0)}_{0d;d0}\mathcal{G}^{(0)}_{dd;dd} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{dd;d0}\right)\mathcal{G}^{(0)}_{d0;0d} \\ \quad\quad \left. + \left(\mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{d0;d0} - \mathcal{G}^{(0)}_{0d;d0}\mathcal{G}^{(0)}_{d0;dd}\right)\mathcal{G}^{(0)}_{dd;0d}\right] \\ \mathcal{G}^{(0)}_{d0;0d} + t_1\left[\mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{0d;0d} + \left(\mathcal{G}^{(0)}_{dd;d0} - \mathcal{G}^{(0)}_{0d;dd}\right)\mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{d0;d0}\mathcal{G}^{(0)}_{dd;0d}\right] \\ \quad +{t_1}^2\left[\left(\mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{dd;d0} - \mathcal{G}^{(0)}_{d0;d0}\mathcal{G}^{(0)}_{dd;dd}\right)\mathcal{G}^{(0)}_{0d;0d} \right.\\ \quad\quad + \left(\mathcal{G}^{(0)}_{0d;d0}\mathcal{G}^{(0)}_{dd;dd} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{dd;d0}\right)\mathcal{G}^{(0)}_{d0;0d} \\ \quad\quad \left. + \left(\mathcal{G}^{(0)}_{d0;d0}\mathcal{G}^{(0)}_{0d;dd} - \mathcal{G}^{(0)}_{0d;d0}\mathcal{G}^{(0)}_{d0;dd}\right)\mathcal{G}^{(0)}_{dd;0d}\right] \\ \mathcal{G}^{(0)}_{dd;0d} + t_1\left[\mathcal{G}^{(0)}_{dd;dd}\mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{dd;dd}\mathcal{G}^{(0)}_{d0;0d} + \left(\mathcal{G}^{(0)}_{d0;dd} - \mathcal{G}^{(0)}_{0d;dd}\right)\mathcal{G}^{(0)}_{dd;0d}\right] \end{pmatrix}, \tag{3.22}$$

$$\begin{pmatrix}\mathcal{G}_{0d;d0}\\ \mathcal{G}_{d0;d0}\\ \mathcal{G}_{dd;d0}\end{pmatrix} = \frac{1}{D}\begin{pmatrix} \mathcal{G}^{(0)}_{0d;d0} + t_1\left[\left(\mathcal{G}^{(0)}_{d0;dd}-\mathcal{G}^{(0)}_{dd;0d}\right)\mathcal{G}^{(0)}_{0d;d0} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{d0;d0} + \mathcal{G}^{(0)}_{0d;0d}\mathcal{G}^{(0)}_{dd;d0}\right] \\ \quad +{t_1}^2\left[\left(\mathcal{G}^{(0)}_{d0;0d}\mathcal{G}^{(0)}_{dd;dd} - \mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{dd;0d}\right)\mathcal{G}^{(0)}_{0d;d0} \right.\\ \quad\quad + \left(\mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{0d;0d}\mathcal{G}^{(0)}_{dd;dd}\right)\mathcal{G}^{(0)}_{d0;d0} \\ \quad\quad \left. + \left(\mathcal{G}^{(0)}_{0d;0d}\mathcal{G}^{(0)}_{d0;dd} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{d0;0d}\right)\mathcal{G}^{(0)}_{dd;d0}\right] \\ \mathcal{G}^{(0)}_{d0;d0} + t_1\left[\mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{0d;d0} - (\mathcal{G}^{(0)}_{dd;0d}+\mathcal{G}^{(0)}_{0d;dd})\mathcal{G}^{(0)}_{d0;d0} + \mathcal{G}^{(0)}_{d0;0d}\mathcal{G}^{(0)}_{dd;d0}\right] \\ \quad +{t_1}^2\left[\left(\mathcal{G}^{(0)}_{d0;0d}\mathcal{G}^{(0)}_{dd;dd} - \mathcal{G}^{(0)}_{d0;dd}\mathcal{G}^{(0)}_{dd;0d}\right)\mathcal{G}^{(0)}_{0d;d0} \right.\\ \quad\quad + \left(\mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{0d;0d}\mathcal{G}^{(0)}_{dd;dd}\right)\mathcal{G}^{(0)}_{d0;d0} \\ \quad\quad \left. + \left(\mathcal{G}^{(0)}_{0d;0d}\mathcal{G}^{(0)}_{d0;dd} - \mathcal{G}^{(0)}_{0d;dd}\mathcal{G}^{(0)}_{d0;0d}\right)\mathcal{G}^{(0)}_{dd;d0}\right] \\ \mathcal{G}^{(0)}_{dd;d0} + t_1\left[\mathcal{G}^{(0)}_{dd;dd}\mathcal{G}^{(0)}_{0d;d0} - \mathcal{G}^{(0)}_{dd;dd}\mathcal{G}^{(0)}_{d0;d0} + (\mathcal{G}^{(0)}_{d0;dd} - \mathcal{G}^{(0)}_{0d;dd})\mathcal{G}^{(0)}_{dd;d0}\right] \end{pmatrix}, \tag{3.23}$$

$$\begin{aligned} D = 1 &- t_1\left(\mathcal{G}^{(0)}_{0d;dd} - \mathcal{G}^{(0)}_{d0;dd} + \mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{dd;d0}\right) \\ &+ {t_1}^2\left[(\mathcal{G}^{(0)}_{0d;dd} - \mathcal{G}^{(0)}_{d0;dd})(\mathcal{G}^{(0)}_{dd;0d} - \mathcal{G}^{(0)}_{dd;d0}) \right.\\ &\quad \left. -(\mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{0d;d0} + \mathcal{G}^{(0)}_{d0;d0})\mathcal{G}^{(0)}_{dd;dd}\right]. \end{aligned} \tag{3.24}$$

Then, the equation corresponding to Eq. (2.24) is given by

$$\begin{aligned} \langle d,d|L_{\rm eff}|d,d\rangle &= {t_1}^2\left(\mathcal{G}_{0d;0d} - \mathcal{G}_{d0;0d} - \mathcal{G}_{0d;d0} + \mathcal{G}_{d0;d0}\right) \\ &= \frac{{t_1}^2}{D}\left(\mathcal{G}^{(0)}_{0d;0d} - \mathcal{G}^{(0)}_{d0;0d} - \mathcal{G}^{(0)}_{0d;d0} + \mathcal{G}^{(0)}_{d0;d0}\right). \end{aligned} \tag{3.25}$$

Thus, the problem is reduced to obtaining the Green's function of $\mathcal{H}_0$.

The Green's function of the two-particle Hamiltonian $\mathcal{H}_0$ is described by the convolution of one-particle Green's functions as follows:

$$\begin{aligned}\langle\alpha,\beta|\frac{1}{z-\mathcal{H}_0}|\alpha',\beta'\rangle &= \frac{1}{2\pi i}\int_{-\infty}^{\infty} dz_a \langle\alpha|\frac{1}{z_a-\mathcal{H}_a}|\alpha'\rangle\langle\beta|\frac{1}{(z-z_a)-\mathcal{H}_b}|\beta'\rangle, \\ &= \frac{1}{2\pi i}\int_{-\infty}^{\infty} \mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a)dz_a, \end{aligned} \tag{3.26}$$

where

$$\mathcal{G}^{(a)}_{\alpha;\alpha'} = \langle\alpha|\frac{1}{z-\mathcal{H}_a}|\alpha'\rangle, \tag{3.27}$$

$$\mathcal{G}^{(a)}_{\beta;\beta'} = \langle\beta|\frac{1}{z-\mathcal{H}_b}|\beta'\rangle. \tag{3.28}$$

$$(\alpha,\alpha'=0,d, \quad \beta,\beta'=0,d). \tag{3.29}$$

The reason why the two-particle Green's function can be described by such form is given in Appendix A.4.

Thus the problem is reduced to obtain the terms

$$\mathcal{G}^{(a)}_{0;0}, \quad \mathcal{G}^{(a)}_{0;d}, \quad \mathcal{G}^{(a)}_{d;0}, \quad \mathcal{G}^{(a)}_{d;d}, \tag{3.30}$$

$$\mathcal{G}^{(b)}_{0;0}, \quad \mathcal{G}^{(b)}_{0;d}, \quad \mathcal{G}^{(b)}_{d;0}, \quad \mathcal{G}^{(b)}_{d;d}. \tag{3.31}$$

As we see in Appendix A.5, we obtain the Green's functions for the particle a as follows:

$$\begin{pmatrix}\mathcal{G}^{(a)}_{0;0} & \mathcal{G}^{(a)}_{0;d} \\ \mathcal{G}^{(a)}_{d;0} & \mathcal{G}^{(a)}_{d;d}\end{pmatrix} = \frac{1}{4it^2\sin k\cos k + {t_1}^2}\begin{pmatrix}2t\cos k & t_1 \\ t_1 & -2it\sin k\end{pmatrix}. \tag{3.32}$$

For obtaining the Green's function for the particle b, we substitute each $-t_1$ and $-t$ for t_1 and t, respectively, and then

$$\mathcal{G}^{(b)}_{\alpha;\alpha'}(k) = -\mathcal{G}^{(a)}_{\alpha;\alpha'}(k), \qquad (\alpha,\alpha'=0,\mathrm{d}). \tag{3.33}$$

In the future work, using the discussion of the present section, we try to obtain the eigenvalues of the Liouvillian rigorously and compare the results with those in Sec. 2.4.

Chapter 4

Summary

In the present thesis, we considered the eigenvalue problem of the Liouvillian of the models which consist of a T-type quantum dot and an infinitely long lead, presented methods of finding nontrivial eigenvalues and showed the nontrivial complex eigenvalues in perturbational analysis.

In Chap. 2, we solved the eigenvalues of the Liouvillian by the perturbation analysis. In Sec. 2.1, we introduced the model, which can have complex eigenvalues of the Hamiltonian after analytic continuation, details of which are in Appendix A.1, as well as the approach, which is called the Feshbach formalism. In Sec. 2.2, we introduced our diagram expansion and showed the evidence for the existence of the nontrivial eigenvalues of the Liouvillian by indicating the simultaneous operation of G_0 on the bra state and ket state. In Sec. 2.3, we showed how to obtain the integral equation corresponding to the original eigenvalue problem of the Liouvillian. In Sec. 2.4, we obtained trivial and nontrivial eigenvalues by the second-order perturbation analysis of the integral equation. We derived the trivial eigenvalues by expanding the domain of the integral after we integrate all terms completely. On the other hand, we derived the nontrivial eigenvalues by expanding the domain of the function which was obtained by integrating only the terms implying the entanglement of the bra state and the ket state.

Our research about complex eigenvalues of the Liouvillian will be completed when we confirm that these nontrivial eigenvalues are physically relevant. A possible method of showing whether the nontrivial eigenvalues are physically relevant or not is to examine the dynamics of the same system numerically. If the complex eigenvalues have the physical meaning, it should describe the relaxation time from a quasi-stable state to the equilibrium state as follows. If ρ_1 is an eigenstate of the Liouvillian and z_1 is the corresponding eigenvalue, we have

$$i\frac{\partial}{\partial t}\rho_1 = z_1\rho_1. \tag{4.1}$$

The equilibrium state ρ_{eq} is also an eigenstate and its eigenvalue z_{eq} is equal to zero. Because the Liouville equation is linear, we have the following solution:

$$\begin{aligned}\rho &= \rho_{\mathrm{eq}} + \rho_1 e^{-i(z_1 - z_{\mathrm{eq}})t} \\ &= \rho_{\mathrm{eq}} + \rho_1 e^{-iz_1 t}.\end{aligned} \tag{4.2}$$

Thus, if z_1 is a complex eigenvalue, the imaginary part of z_1 is the inverse relaxation time. In the future, we examine the dynamics of the Liouvillian and whether the complex eigenvalues which we obtained in Sec. 2.4 describe the relaxation time or not.

In Chap. 3, we introduced the method of solving the eigenvalue problem of the Liouvillian rigorously. In Sec. 3.1, we showed the powerfulness of this method by expanding the model that we treat. In Sec. 3.2, using this method we tried to obtain the eigenvalues of the Liouvillian rigorously. It was not a simple calculation, and unfortunately we have not achieved the solution. However, this method may be an easy methodology of obtaining the relaxation time.

Appendix A

A.1 The spectrum of the one-dot model by the Feshbach formalism

In this Appendix, we introduce a formalism called the Feshbach formalism, which is equivalent to the Schrödinger equation. The Shrödinger equation is the following:

$$H|\phi\rangle = E|\phi\rangle, \tag{A.1}$$

which is equivalent to the following:

$$H\left(P_{\mathrm{s}} + Q_{\mathrm{s}}\right)|\phi\rangle = E\left(P_{\mathrm{s}} + Q_{\mathrm{s}}\right)|\phi\rangle, \tag{A.2}$$

where P_{s} is the projector on a system in question, Q_{s} is a projector on an environment, and

$$P_{\mathrm{s}} + Q_{\mathrm{s}} = I_{\mathrm{s}}, \tag{A.3}$$

where I_{s} is the identity operator in the Hilbert space. Operating P_{s} and Q_{s} from the left, we can transform Eq. (A.2) as

$$P_s H\left(P_s + Q_s\right)|\phi\rangle = EP_s|\phi\rangle, \tag{A.4}$$

$$Q_s H\left(P_s + Q_s\right)|\phi\rangle = EQ_s|\phi\rangle. \tag{A.5}$$

Then we have

$$P_s|\phi\rangle = \frac{1}{E - P_s H P_s} P_s H Q_s|\phi\rangle, \tag{A.6}$$

$$Q_s|\phi\rangle = \frac{1}{E - Q_s H Q_s} Q_s H P_s|\phi\rangle. \tag{A.7}$$

Substituting Eq. (A.7) into Eq. (A.4) and Eq. (A.6) into Eq. (A.5), we obtain the following equations equivalent to the Shrödinger equation:

$$\left[P_s H P_s + P_s H Q_s \frac{1}{E - Q_s H Q_s} Q_s H P_s\right] P_s|\phi\rangle = EP_s|\phi\rangle, \tag{A.8}$$

$$\left[Q_s H Q_s + Q_s H P_s \frac{1}{E - P_s H P_s} P_s H Q_s\right] Q_s|\phi\rangle = EQ_s|\phi\rangle. \tag{A.9}$$

In the present thesis, we use only Eq. (A.8) because it contains the information of the eigenvalues that are our first aim.

Using Eq. (A.8), we derive the solution of the eigenvalue problem of the Hamiltonian:

$$H = -t\sum_{-\infty}^{\infty}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) - t_1(c_d^\dagger c_0 + c_0^\dagger c_d), \tag{A.10}$$

where $c_x^\dagger$ and c_x are the creation and annihilation operators at the site x on the lead, respectively, while $c_d^\dagger$ and c_d are those at the dot. Our aim here is to solve the eigenvalue problem (A.1) using the Feshbach formalism. We can express Eq.(A.8) in the form

$$H_{\text{eff}}(E)(P_{\text{s}}|\phi\rangle) = E(P_{\text{s}}|\phi\rangle), \tag{A.11}$$

where

$$H_{\text{eff}}(E) = P_{\text{s}}HP_{\text{s}} + P_{\text{s}}HQ_{\text{s}}\frac{1}{E - Q_{\text{s}}HQ_{\text{s}}}Q_{\text{s}}HP_{\text{s}}. \tag{A.12}$$

For the Hamiltonian (A.10), we have

$$P_{\text{s}}HP_{\text{s}} = 0, \tag{A.13}$$

$$P_{\text{s}}HQ_{\text{s}} = -t_1 c_d^\dagger c_0, \tag{A.14}$$

$$Q_{\text{s}}HP_{\text{s}} = -t_1 c_0^\dagger c_d, \tag{A.15}$$

$$Q_{\text{s}}HQ_{\text{s}} = -t\sum_{-\infty}^{\infty}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x). \tag{A.16}$$

We need only one element of $H_{\text{eff}}(E)$ to solve Eq. (A.11). The eigenvalue problem is now reduced to

$$\langle d|H_{\text{eff}}|d\rangle = -t_1^2\langle 0|\frac{1}{E - Q_{\text{s}}HQ_{\text{s}}}|0\rangle = E, \tag{A.17}$$

where

$$\begin{aligned}
\langle 0|\frac{1}{E - Q_{\text{s}}HQ_{\text{s}}}|0\rangle &= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\langle 0|k\rangle\langle k|\frac{1}{E - Q_{\text{s}}HQ_{\text{s}}}|k\rangle\langle k|0\rangle \\
&= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{1}{E + 2t\cos k} \\
&= \int_{-\infty}^{\infty}\frac{1}{2\pi}\frac{dx}{1+x^2}\frac{1}{E + 2t\frac{1-x^2}{1+x^2}} \\
&= \int_{-\infty}^{\infty}\frac{2dx}{2\pi(E-2t)}\frac{1}{(x - \sqrt{-\frac{E+2t}{E-2t}})(x + \sqrt{-\frac{E+2t}{E-2t}})} \\
&= \pm\frac{i}{(E-2t)\sqrt{-\frac{E+2t}{E-2t}}},
\end{aligned} \tag{A.18}$$

and

$$\mathrm{Re}\sqrt{\alpha} > 0 \tag{A.19}$$

for arbitrary α. In the third line of Eq. (A.18) we transformed the variable as $x = \tan k/2$. In the sixth line of Eq. (A.18), we should take the upper sign if

$$\mathrm{Im}\sqrt{-\frac{E+2t}{E-2t}} > 0, \tag{A.20}$$

and the lower sign otherwise.

In what follows, we consider the case of (A.20). The original eigenvalue problem (A.17) is the following:

$$E = \frac{i}{(E-2t)\sqrt{-\frac{E+2t}{E-2t}}}. \tag{A.21}$$

The solution is given by

$$E^2 = 2t^2 \pm \sqrt{4t^4 + t_1^4}. \tag{A.22}$$

Transforming Eq. (A.21), we obtain the relation

$$\sqrt{-\frac{E+2t}{E-2t}} = \frac{i}{E(E-2t)}. \tag{A.23}$$

If we take the lower-sign solution of Eq. (A.22), the imaginary part of the left-hand side of Eq. (A.23) is negative, and then it conflicts with the condition (A.20). On the other hand, the upper-sign solution of Eq. (A.22) does not conflict with the condition (A.20). Then the correct solution of Eq. (A.17) is the following:

$$E = \pm\sqrt{2t^2 + \sqrt{4t^4 + t_1^4}}. \tag{A.24}$$

Next, we discuss the lower-sign solution of Eq. (A.22):

$$E = \pm i\sqrt{\sqrt{4t^4 + t_1^4} - 2t^2}. \tag{A.25}$$

They are not in the domain of the right-hand side of (A.21) and we should not take them as the solution of Eq. (A.21). However, these 'solutions' have physical meaning. We can interpret them as the eigenvalues that appear when we do the analytic continuation of the right-hand side of Eq. (A.21) to the other region of (A.20). In general, these eigenvalues are complex, the corresponding eigenstates describe physically relevant quasi-stable states, and the inverse of the imaginary part of the complex eigenvalues are the lifetime of the quasi-stable states; see Appendix A.2 for details.

A.2 Physical meanings of complex eigenvalues of the Hamiltonian

In the present Appendix, we explain the physical meaning of complex eigenvalues of the Hamiltonian, following Ref. [2]. As we discuss in the following, the imaginary parts of the complex eigenvalues describe the lifetime and the momentum flux.

In the following discussion, we consider the case of one dimension:

$$\hat{\mathcal{H}} = \hat{\mathcal{K}} + \hat{\mathcal{V}}, \tag{A.26}$$

$$\hat{\mathcal{K}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, \tag{A.27}$$

$$\hat{\mathcal{V}} = V(x), \tag{A.28}$$

where $V(x)$ has a finite support:

$$\Omega_{\rm pot} := \{x| -l \leq x \leq l\}, \tag{A.29}$$

and Hermitian: $V(x)^* = V(x)$.

For discussing the case of an arbitrary wave function $\phi(x)$ which may not be restricted to the Hilbert space, we define the quantity

$$\langle\psi|\mathcal{H}|\psi\rangle_\Omega := \int_{-L}^{L} \psi^*(x)\hat{\mathcal{H}}\psi(x)dx, \tag{A.30}$$

where

$$\Omega := \{x| -L \leq x \leq L\} \tag{A.31}$$

with $L > l$. Then we can define the expectation value

$$\langle\psi|\hat{\mathcal{H}}|\psi\rangle := \lim_{|\Omega|\to\infty} \frac{\langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega}{\langle\psi|\psi\rangle_\Omega}. \tag{A.32}$$

Now we focus on the imaginary part of $\langle\psi|\hat{\mathcal{H}}|\psi\rangle$. We suppose that $|\psi\rangle$ is not restricted to the element of the Hilbert space. Then we show below that

$$2i{\rm Im}\langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega = \langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega - (\langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega)^*, \tag{A.33}$$

can be nonzero. The potential function is a real and localized function, and therefore the expectation value of the potential must be real. Thus the imaginary part of the element $\langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega$ is equal to the imaginary part of the expectation value of the kinetic term:

$$\begin{aligned}
{\rm Im}\langle\psi|\hat{\mathcal{H}}|\psi\rangle_\Omega &= {\rm Im}\langle\psi|\hat{\mathcal{K}}|\psi\rangle_\Omega, \\
&= {\rm Im}\left(-\frac{\hbar^2}{2m}\int_{-L}^{L}\psi^*(x)\psi''(x)dx\right), \\
&= {\rm Im}\left(\frac{\hbar^2}{2m}\int_{-L}^{L}\psi'(x)^*\psi'(x)dx - \frac{\hbar^2}{2m}[\psi(x)^*\psi'(x)]_{-L}^{L}\right), \\
&= {\rm Im}\left(-\frac{\hbar^2}{2m}\left[\psi(x)^*\psi'(x)\right]_{-L}^{L}\right), \\
&= -\frac{\hbar}{2m}{\rm Re}\left[\psi(x)^*\hat{p}\psi(x)\right]_{-L}^{L},
\end{aligned} \tag{A.34}$$

where $\hat{p}$ is the momentum operator, and in the third line, we used the fact that the first term is a norm and then is positive while the second part can be complex. Equation (A.34) shows that the imaginary part of the expectation value is proportional to the momentum flux out of the segment Ω.

Hereafter we discuss the relation between the imaginary part of a complex eigenvalue and the lifetime of the state, using the time-dependent Shrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{\mathcal{H}}\Psi(x,t). \tag{A.35}$$

The particle number in the segment Ω is given by

$$N_\Omega(t) := \langle\Psi|\Psi\rangle_\Omega. \tag{A.36}$$

Then its time derivative is given by

$$\begin{aligned}
\frac{d}{dt}N_\Omega(t) &= \int_{-L}^{L}\left(\Psi(x,t)^*\frac{\partial\Psi(x,t)}{\partial t} + \frac{\partial\Psi(x,t)^*}{\partial t}\Psi(x,t)\right)dx \\
&= -\frac{i}{\hbar}\int_{-L}^{L}\left[\Psi(x,t)^*\hat{\mathcal{H}}\Psi(x,t) - \left(\hat{\mathcal{H}}\Psi(x,t)\right)^*\Psi(x,t)\right]dx \\
&= \frac{2}{\hbar}\mathrm{Im}\langle\Psi|\hat{\mathcal{H}}|\Psi\rangle_\Omega,
\end{aligned} \tag{A.37}$$

where we used the time-dependent Schrödinger equation and its conjugate. Equation (A.37) shows that the imaginary part of a complex eigenvalue describes the lifetime of the particle number in the system.

Thus we conclude that the imaginary part of a complex eigenvalue has two physical meanings; one is the momentum flux and the other is the lifetime.

A.3 The Liouville space

In the present Appendix, we introduce some properties and notations for simplicity of calculations. In the Liouville space, the operators are cumbersome to treat. The following notations are convenient for calculations.

The Liouville space consists of density matrices ρ and is a Hilbert space with an inner product $\langle\langle\alpha'\beta'|\alpha\beta\rangle\rangle$ defined as follows:

$$|\alpha,\beta\rangle\rangle := |\alpha\rangle\langle\beta|, \quad \{|\alpha\rangle\} \ : \ \text{CONS}, \tag{A.38}$$

$$\rho = \sum_{\alpha,\beta} c_{\alpha\beta}|\alpha,\beta\rangle\rangle, \tag{A.39}$$

$$\begin{aligned}
L|\alpha,\beta\rangle\rangle &= [H,|\alpha\rangle\langle\beta|] = (E_\alpha - E_\beta)|\alpha\rangle\langle\beta| \\
&= (E_\alpha - E_\beta)|\alpha,\beta\rangle\rangle,
\end{aligned} \tag{A.40}$$

$$\langle\langle\alpha',\beta'|\alpha,\beta\rangle\rangle := \mathrm{tr}[(|\alpha'\rangle\langle\beta'|)^\dagger(|\alpha\rangle\langle\beta|)] = \delta_{\alpha\alpha'}\delta_{\beta'\beta}, \tag{A.41}$$

$$I = \sum_{\alpha,\beta}|\alpha,\beta\rangle\rangle\langle\langle\alpha,\beta|, \tag{A.42}$$

where I is the identity operator in the Liouville space. Throughout the thesis, the operators that are denoted by capital letters without subscripts are in the Liouville space and

operate on density matrices, while those with the subscript 's' operate on state vectors of the original Hilbert space. For simplification, we introduce the operation '$\times$' as follows:

$$
\begin{aligned}
(A_{\rm s} \times B_{\rm s})\rho &:= A_s \rho B_{\rm s}, && \text{(A.43)}\\
A_{\rm s} \times (bB_{\rm s} + cC_{\rm s}) &= bA_{\rm s} \times B_{\rm s} + cA_{\rm s} \times C_{\rm s}, && \text{(A.44)}\\
(bB_{\rm s} + cC_{\rm s}) \times A_{\rm s} &= bB_{\rm s} \times A_{\rm s} + cC_{\rm s} \times A_{\rm s}, && \text{(A.45)}\\
(A_{\rm s} \times 0)\rho &= 0 = (0 \times B_{\rm s})\rho, && \text{(A.46)}\\
(C_{\rm s} \times D_{\rm s})(A_{\rm s} \times B_{\rm s}) &= C_{\rm s}A_{\rm s} \times B_{\rm s}D_{\rm s}, && \text{(A.47)}
\end{aligned}
$$

where ρ is a density matrix and b and c are c-numbers. Then the Liouvillian is given by

$$
L = H \times I_{\rm s} - I_{\rm s} \times H, \tag{A.48}
$$

where $I_{\rm s}$ is the identity operator in the original Hilbert space, because then we have

$$
L\rho = H\rho - \rho H = [H, \rho]. \tag{A.49}
$$

We also define the projection operators

$$
\begin{aligned}
P &:= P_{\rm s} \times P_{\rm s}, && \text{(A.50)}\\
Q &:= Q_{\rm s} \times Q_{\rm s} + P_{\rm s} \times Q_{\rm s} + Q_{\rm s} \times P_{\rm s}, && \text{(A.51)}\\
P &+ Q = I, && \text{(A.52)}\\
P_{\rm s} &+ Q_{\rm s} = I_{\rm s}, && \text{(A.53)}
\end{aligned}
$$

where P and $P_{\rm s}$ are the projections on the main system and Q and $Q_{\rm s}$ are the projections on the environment in the respective space.

A.4 The relationship between two-particle Hamiltonian and one-particle Hamiltonian

In the present appendix, we show that the Green's function of two independent distinguishable particles is given by the convolution of one-particle Green's functions.

Let us consider a two-particle Hamiltonian:

$$
\mathcal{H}_0 = \mathcal{H}_a + \mathcal{H}_b, \tag{A.54}
$$

where $\mathcal{H}_a$ is the Hamiltonian of the particle a and $\mathcal{H}_b$ is the Hamiltonian of the particle b. The Green's function of two distinguishable particles is written as

$$
\begin{aligned}
\langle \alpha, \beta | \frac{1}{z - \mathcal{H}_0} | \alpha', \beta' \rangle &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz_a \langle \alpha | \frac{1}{z_a - \mathcal{H}_a} | \alpha' \rangle \langle \beta | \frac{1}{(z - z_a) - \mathcal{H}_b} | \beta' \rangle \\
&= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a) \mathcal{G}^{(b)}_{\beta;\beta'}(z - z_a) dz_a, \qquad \text{(A.55)}
\end{aligned}
$$

where

$$\mathcal{G}^{(a)}_{\alpha;\alpha'} = \langle\alpha|\frac{1}{z-\mathcal{H}_a}|\alpha'\rangle, \tag{A.56}$$

$$\mathcal{G}^{(a)}_{\beta;\beta'} = \langle\beta|\frac{1}{z-\mathcal{H}_b}|\beta'\rangle, \tag{A.57}$$

$$(\alpha,\alpha'=0,d, \quad \beta,\beta'=0,d),$$

and

$$\mathcal{G}^{(0)}_{\alpha\beta;\alpha'\beta'} = \langle\alpha,\beta|\frac{1}{z-\mathcal{H}_0}|\alpha',\beta'\rangle \tag{A.58}$$

$$(\alpha,\alpha'=0,d, \quad \beta,\beta'=0,d).$$

We show Eq. (A.55) in the following.

The Green's functions are originally defined as the solution of the following equations:

$$\left((z-\mathcal{H}_0)\mathcal{G}^{(0)}(z)\right)_{\alpha\beta;\alpha'\beta'} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}, \tag{A.59}$$

$$\left((z-\mathcal{H}_a)\mathcal{G}^{(a)}(z)\right)_{\alpha\alpha'} = \delta_{\alpha\alpha'}, \tag{A.60}$$

$$\left((z-\mathcal{H}_b)\mathcal{G}^{(b)}(z)\right)_{\beta;\beta'} = \delta_{\beta\beta'}. \tag{A.61}$$

Applying $(z-\mathcal{H}_0)$ from the left of the right-hand side of Eq. (A.55), we have

$$\begin{aligned}
&\frac{1}{2\pi i}\left((z-\mathcal{H}_0)\int_{-\infty}^{\infty}\mathcal{G}^{(a)}(z_a)\mathcal{G}^{(b)}(z-z_a)dz_a\right)_{\alpha\beta;\alpha'\beta'} \\
&= \frac{1}{2\pi i}\int_{-\infty}^{\infty}dz_a\Big[z\mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a) \\
&\qquad -\left(\mathcal{H}_a\mathcal{G}^{(a)}(z_a)\right)_{\alpha;\alpha'}\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a) - \mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\left(\mathcal{H}_b\mathcal{G}^{(b)}(z-z_a)\right)_{\beta;\beta'}\Big] \\
&= \frac{1}{2\pi i}\int_{-\infty}^{\infty}dz_a\Big[z\mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a) \\
&\qquad +\Big(\delta_{\alpha\alpha'} - z_a\mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a) \\
&\qquad +\mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\left(\delta_{\beta\beta'} - (z-z_a)\,\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a)\right)\Big)\Big] \\
&= \frac{1}{2\pi i}\int_{-\infty}^{\infty}dz_a\left[\delta_{\alpha\alpha'}\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a) + \mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)\delta_{\beta\beta'}\right],
\end{aligned} \tag{A.62}$$

where we used Eqs. (A.60) and (A.61) in the second line. Thus, showing Eq. (A.55) is reduced to showing the following equations:

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathcal{G}^{(a)}_{\alpha;\alpha'}(z_a)dz_a = \frac{1}{2}\delta_{\alpha\alpha'}, \tag{A.63}$$

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathcal{G}^{(b)}_{\beta;\beta'}(z-z_a)dz_a = \frac{1}{2}\delta_{\beta\beta'}. \tag{A.64}$$

Now, we derive Eqs. (A.63) and (A.64). The Green's function is the Fourier transformation of the propagator:

$$\mathcal{G}^{(a)}_{\alpha;\alpha'}(z-i\eta) = i\int_{-\infty}^{0} dt e^{i(z-i\eta)t}\left(e^{-i\mathcal{H}_a t}\right)_{\alpha;\alpha'}, \tag{A.65}$$

$$\mathcal{G}^{(b)}_{\beta;\beta'}(z-i\eta) = i\int_{-\infty}^{0} dt e^{i(z-i\eta)t}\left(e^{-i\mathcal{H}_b t}\right)_{\beta;\beta'}. \tag{A.66}$$

The expression (A.65) indeed satisfies Eq. (A.59):

$$\begin{aligned}\left((z-i\eta-\mathcal{H}_a)\,\mathcal{G}^{(a)}(z-i\eta)\right)_{\alpha;\alpha'} &= i\int_{-\infty}^{0} dt\left((z-i\eta-\mathcal{H}_a)\,e^{i(z-i\eta-\mathcal{H}_a)t}\right)_{\alpha;\alpha'}\\ &= \int_{-\infty}^{0} dt\left(\frac{d}{dt}e^{i(z-i\eta-\mathcal{H}_a)t}\right)_{\alpha;\alpha'}\\ &= \left(e^{i(z-i\eta-\mathcal{H}_a)t}\right)_{\alpha;\alpha'}\Big|_{t=-\infty}^{0}\\ &= \delta_{\alpha\alpha'}.\end{aligned} \tag{A.67}$$

Integrating Eq. (A.65) with respect to z, we obtain

$$\begin{aligned}\int_{-\infty}^{\infty}\mathcal{G}^{(a)}_{\alpha;\alpha'}(z-i\eta)dz &= i\int_{-\infty}^{\infty}dz\int_{-\infty}^{0}dt e^{i(z-i\eta)t}\left(e^{-i\mathcal{H}_a t}\right)_{\alpha;\alpha'}\\ &= i\int_{-\infty}^{0}dt\int_{-\infty}^{\infty}dz e^{i(z-i\eta)t}\left(e^{-i\mathcal{H}_a t}\right)_{\alpha;\alpha'}\\ &= 2\pi i\int_{-\infty}^{0}dt\delta(t)e^{\eta t}\left(e^{-i\mathcal{H}_a t}\right)_{\alpha;\alpha'}.\end{aligned} \tag{A.68}$$

Thus we arrive at

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathcal{G}^{(a)}_{\alpha;\alpha'}(z-i\eta)dz = \frac{1}{2}\delta_{\alpha\alpha'}, \tag{A.69}$$

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathcal{G}^{(b)}_{\beta;\beta'}(z-i\eta)dz = \frac{1}{2}\delta_{\beta\beta'}, \tag{A.70}$$

which give Eqs. (A.63) and (A.64).

A.5 The Green's function of the one-dot model

Let us derive the element of the Green's function of the one-dot model:

$$H = H_0 + H_1,$$

$$H_0 = -t\sum_{x=-\infty}^{\infty}(c^\dagger_{x+1}c_x + c^\dagger_x c_{x+1}), \tag{A.71}$$

$$H_1 = -t_1(d^\dagger c_0 + c^\dagger_0 d). \tag{A.72}$$

We derive the following terms:

$$\langle d|\frac{1}{E-H}|d\rangle, \quad \langle d|\frac{1}{E-H}|0\rangle,$$
$$\langle 0|\frac{1}{E-H}|d\rangle, \quad \langle 0|\frac{1}{E-H}|0\rangle.$$

Using the Dyson equation, we obtain the following closed equations:

$$\begin{aligned}
\langle d|\frac{1}{E-H}|0\rangle &= \langle d|\frac{1}{E-H_0}H_1\frac{1}{E-H}|0\rangle \\
&= \langle d|\frac{1}{E-H_0}|d\rangle\langle d|H_1|0\rangle\langle 0|\frac{1}{E-H}|0\rangle \\
&= -\frac{t_1}{E}\langle 0|\frac{1}{E-H}|0\rangle, \qquad \text{(A.73)} \\
\langle 0|\frac{1}{E-H}|0\rangle &= \langle 0|\frac{1}{E-H_0}|0\rangle \\
&+ \langle 0|\frac{1}{E-H_0}|0\rangle\langle 0|H_1|d\rangle\langle d|\frac{1}{E-H}|0\rangle \\
&= \langle 0|\frac{1}{E-H_0}|0\rangle \\
&- t_1\langle 0|\frac{1}{E-H_0}|0\rangle\langle d|\frac{1}{E-H}|0\rangle. \qquad \text{(A.74)}
\end{aligned}$$

Let us define

$$A(E) = -\frac{t_1}{E}\langle 0|\frac{1}{E-H_0}|0\rangle. \qquad \text{(A.75)}$$

Then we obtain

$$\langle 0|\frac{1}{E-H}|0\rangle = \frac{-EA(E)}{t_1(1+t_1A(E))}, \qquad \text{(A.76)}$$
$$\langle 0|\frac{1}{E-H}|0\rangle = \frac{A(E)}{t_1(1+t_1A(E))}. \qquad \text{(A.77)}$$

The dispersion relation in this case is the following:

$$E = -2t\cos k, \qquad \text{(A.78)}$$

and we use the upper sign of the following equation:

$$\begin{aligned}
\langle 0|\frac{1}{E-H_0}|0\rangle &= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\langle 0|k\rangle\langle\frac{1}{E-H_0}|k\rangle\langle k|0\rangle \\
&= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{1}{E+2t\cos k} \\
&= \pm\frac{i}{(E-2t)\sqrt{-\frac{E+2t}{E-2t}}}. \qquad \text{(A.79)}
\end{aligned}$$

Then we obtain

$$\langle d|\frac{1}{E-H}|0\rangle = \frac{t_1}{4it^2\sin k\cos k + t_1^2}, \tag{A.80}$$

$$\langle 0|\frac{1}{E-H}|0\rangle = \frac{2t\cos k}{4it^2\sin k\cos k + t_1^2}. \tag{A.81}$$

In the same way, we obtain

$$\langle d|\frac{1}{E-H}|d\rangle = \frac{-2it\sin k}{4it^2\sin k\cos k + t_1^2}, \tag{A.82}$$

$$\langle 0|\frac{1}{E-H}|d\rangle = \frac{t_1}{4it^2\sin k\cos k + t_1^2}. \tag{A.83}$$

Acknowledgements

The author thanks Mr. Takashi Mori for a tremendous contribution in solving the integral equations and giving insightful comments on the present research totally. A discussion with him lead her to the main results in Sec. 2.4.

The author also thanks Prof. Akinori Nishino. He gave a comment at an early stage of the present research that became the core of the the present research, which was the fact that the eigenvalue problem of the one-particle Liouvillian is reduced to the eigenvalue problem of the two-particle Hamiltonian. Owing to his comment, we were able to obtain the integral equations and introduce the method of solving the eigenvalue problem of the Liouvillian rigorously.

The author appreciates Prof. Tomio Petrosky for total advice. He gave her constructive comments especially about the background of the present research and warm encouragement when he visited the Hatano laboratory.

Finally, she is deeply grateful to Prof. Naomichi Hatano, who is the supervisor. He has been greatly tolerant and supportive and given the great contribution of the whole content of the present research. In particular, she appreciates the fact that he gave such an interesting theme.

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