MASTER THESIS

# Analysis of Resonant States using Non-Hermitian Hamiltonians

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# 論 文 要 旨
## （和　文）

（論文題目）

# 非エルミートなハミルトニアンを用いた共鳴状態の解析

（内容の要旨）

　ある特定のエネルギー（共鳴準位）を持った電子が、量子ドットなどのメゾスコピックな素子に入射すると、ある程度長い時間ドット内に閉じ込められるという現象が起こる。これは一種の共鳴散乱と捉えることができる。

　この類の散乱現象を開放系の定常状態問題として扱うと、共鳴状態における波動関数は遠方で発散するため、数値計算が困難となる。

　我々は、この波動関数と複素数のエネルギー固有値を具体的に求めるために、複素ゲージ変換を施した非エルミートなハミルトニアンを用いる新しい方法を提案する。従来は複素スケーリング法と呼ばれる手法が使われてきたが、この方法には、スケール変換する領域においてポテンシャルが少なくとも解析的でなければ使えない、という制約があった。複素ゲージ変換にはそのような限界がなく、非常に広汎にわたる問題に対して適用が可能である。

　本研究においては、共鳴状態を与えるポテンシャル模型として一次元の井戸型ポテンシャルと、ガウス関数を２つ組み合わせたポテンシャルを扱った。

　前者の問題については、適切な境界条件の下でシュレーディンガー方程式を解くことにより、複素ゲージ変換を用いることなく共鳴状態の波動関数と寿命を求めた。

　後者の問題については、非エルミートなハミルトニアンの固有関数を調和振動子の固有関数であるエルミート多項式で展開し、共鳴エネルギーと寿命を行列の複素固有値として直接求めた。結果として、連続空間模型を扱うことにより、格子模型では求めるのが困難であった共鳴点を比較的精度よく得られることが示された。

Graduate College of Science and Engineering, Aoyama Gakuin University

# Master Thesis
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We propose the use of a novel type of non-Hermitian Hamiltonian for calculating the resonant wave functions and corresponding complex energy eigenvalues concretely. The method of complex scaling has been conventionally used. However, there is a limitation in its applicability. In contrast, the present method of the imaginary gauge transformation is general and can be applicable to extensive problems.

In the present study, we treat two types of the potential, a one-dimensional square well and a combination of two Gaussian functions. In the former problem, we obtained the resonant wave functions and its lifetime by solving the Schrödinger equation under an appropriate boundary conditions without the help of the imaginary gauge transformation. In the latter problem, we obtained the resonant energy and the lifetime directly as complex eigenvalues of a non-Hermitian matrix. We claim that the imaginary gauge transformation provides a unique way of defining resonant states.

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March 26, 2002

**Abstract**

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1

# Contents

# 1 Introduction

Resonant scattering is one of the most interesting phenomena in quantum physics. A well-known example is the Ramsauer-Townsent effect, which gives anomalously large transmission in the scattering of low-energy electrons. Resonant behavior can also emerge when a photon is scattered by an atom in its ground state if the incident energy of the photon is equal to the excitation energy of the atom. In this case, the scattering amplitude shows a very sharp peak.

In fact, the resonance is an intrinsic feature of general open quantum systems. In recent years, the conduction properties of mesoscopic systems have been studied both theoretically and experimentally [1, 2]. Among others, in ballistic transport regime, the effects of the resonance are actually observed [3, 4]. This phenomenan is known as resonance trapping. The energy dependence of the conductance is strongly affected by this effect. However, a general theory that can clarify how the resonance contributes to the conductance has not been constructed yet. The crucial difficulty lies in the treatment of the open systems.

The Hamiltonian of an open quantum system is fundamentally non-Hermitian because the probability density does not need to be conserved. Many theoretical studies of non-Hermitian systems have been made in the framework of different models. In particular, the computation of the resonant states is performed by the method of complex scaling, mainly in the context of nuclear physics [5, 6].

In the present thesis, we propose the use of a new type of non-Hermitian Hamiltonian for the measurement of the location and width of resonant states. This Hamiltonian contains an imaginary vector potential, which plays a very important role in separating the resonant states from the continuum of the scattering states. In addition, in contrast to the optical model, this model precisely reflects the actual scalar potential. The imaginary vector potential was introduced originally in the study of the Anderson localization and has made rapid progress in this field [7–10], whereas it has been hardly used in the study of open quantum systems including mesoscopic systems [11].

In Sec. 2, the physical meaning of the non-Hermiticity is briefly reviewed. We emphasize the importance of boundary conditions. Sec. 3 shows a simple example of resonant scattering. The numerical results are also presented. In Sec. 4, a general theory of the imaginary gauge transformation is formulated. This theory provides a unique way of defining the resonant states. In Sec. 5,

the imaginary gauge transformation is applied to a one-dimensional system and the numerical results are discussed. Finally in Sec. 6, concluding remarks are given.

## 2 Non-Hermiticity of Hamiltonian

In the present section, we review how the Hermiticity of the Hamiltonian depends on boundary conditions. The physical meaning of the complex eigenvalues is mentioned as well.

### 2.1 Boundary Condition for Open Quantum Systems

The usual time-independent Hamiltonian describing stationary states is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}), \tag{2.1}$$

where the potential $V(\mathbf{x})$ is real. Whether this Hamiltonian is Hermitian or not depends on boundary conditions imposed on its eigenfunctions.

If $\mathcal{H}$ is Hermitian, the following equality must hold for an arbitrary state $\phi(\mathbf{x})$:

$$\int \phi^*\mathcal{H}\phi d\mathbf{x} = \int (\mathcal{H}\phi)^*\phi d\mathbf{x}. \tag{2.2}$$

Here the integration is done over the entire region that we are interested in. This is none other than the definition of the Hermitian operator. Of course, the eigenvalues must be real in this case. Using the identity for arbitrary scalar fields $f$ and vector fields $\mathbf{A}$,

$$\nabla \cdot (f\mathbf{A}) = \mathbf{A} \cdot \nabla f + f\nabla \cdot \mathbf{A}, \tag{2.3}$$

we rewrite Eq. (2.2) as follows:

$$\int \nabla \cdot (\phi^*\nabla\phi - \phi\nabla\phi^*)d\mathbf{x} = 0. \tag{2.4}$$

From Gauss's theorem, we can convert this volume integral to the surface integral,

$$\int_S (\phi^*\nabla\phi - \phi\nabla\phi^*) \cdot d\mathbf{S} = 0, \tag{2.5}$$

where $S$ denotes a closed surface enclosing the sufficiently large region and $d\mathbf{S}$ is the surface element vector. Therefore, the Hermiticity (2.2) is equivalent to the boundary condition (2.5). Actually, this condition holds in most cases. For this reason, the Hamiltonian (2.1) is generally treated as a Hermitian operator.

In the following, we consider a one-dimensional space, in paticular. If we define all wave functions $\{\phi(x)\}$ within a large box of length $L$, the Hermiticity condition (2.5) can be written in the form

$$\lim_{L\to\infty}\left[\phi^*\frac{d\phi}{dx}-\frac{d\phi^*}{dx}\phi\right]_{-L/2}^{L/2}=0. \tag{2.6}$$

Needless to say, for bound states, the condition (2.6) holds obviously because its boundary condition is $\phi(\infty)=\phi(-\infty)=0$. Moreover, for a free particle with the periodic boundary condition $\phi(x)=\phi(x+L)$, the condition (2.6) holds as well. Let us also consider the important boundary condition that is used frequently in scattering problem:

$$\phi(x)\sim e^{ikx}+Re^{-ikx}\qquad\text{as}\quad x\to-\infty, \tag{2.7}$$

and

$$\phi(x)\sim Te^{ikx}\qquad\text{as}\quad x\to\infty, \tag{2.8}$$

where $R$ and $T$ are the reflection and transmission coefficient respectively and the wave number $k$ is assumed to be real. If the scattering potential is localized near $x=0$, we can prove the Hermiticity of the Hamiltonian (2.1). Consequently, under all these three types of boundary conditions, which appear commonly in quantum mechanics, the Hamiltonian (2.1) should be Hermitian.

However, if we remove the incident wave $e^{ikx}$ from the boundary condition (2.7), the Hermiticity condition (2.6) does not hold any longer. Therefore, when we adopt the boundary condition

$$\phi(x)\sim e^{ik|x|}\qquad\text{as}\quad |x|\to\infty, \tag{2.9}$$

the Hamiltonian (2.1) is non-Hermitian. This boundary condition is appropriate for describing a scattering state in an open quantum system, since this well expresses the situation that an incident particle eventually goes through the potential barriers.

## 2.2 Physical Meaning of the Complex Energy Eigenvalues

Because of the non-Hermiticiy, the energy eigenvalues $E$ are generally complex under the boundary condition (2.9). Furthermore, the corresponding eigenfunctions are not square-integrable. Assuming that the relation $E = \hbar^2 k^2 / 2m$ is valid far away from the scattering potential, the wave number $k$ must be also complex. Let us write the complex energy and the complex wave number as

$$E = E_r - i\frac{\Gamma}{2}, \qquad (2.10)$$

$$k = k_r - i\gamma, \qquad (2.11)$$

where $E_r$, $\Gamma$, $k_r$, and $\gamma$ are related to each other as follows:

$$E_r = \frac{\hbar^2(k_r^2 - \gamma^2)}{2m}, \qquad (2.12)$$

and

$$\Gamma = \frac{2\hbar^2 k_r \gamma}{m}. \qquad (2.13)$$

Then we have the wave function

$$\phi(x) \sim e^{ik_r|x|+\gamma|x|}, \qquad (2.14)$$

which is diverging as $|x| \to \infty$. Conversely, if we allow divergent functions as solutions of the Schrödinger equation, the corresponding eigenvalues are generally complex as we explained in Sec. 2.1.

The real part of the energy, (2.12), gives the resonant level. Substituting Eq. (2.10) in the time-dependent factor of the stationary state $e^{-iEt/\hbar}$, we have the wave function of the energy eigenstate in the form

$$\Phi_E(x,t) = \phi_E(x)e^{-iE_r t/\hbar}e^{-\Gamma t/2\hbar}. \qquad (2.15)$$

By taking the squared magnitude of the both sides of Eq. (2.15), we obtain the probability density

$$|\Phi_E(x,t)|^2 = |\phi_E(x)|^2 e^{-\Gamma t/\hbar}. \qquad (2.16)$$

Thus the quantity $\hbar/\Gamma$ yields the lifetime of the eigenstate corresponding to the eigenvalue $E$. The lifetime is infinite if the Hamiltonian is Hermitian, i.e. if $\Gamma = 0$.

# 3 A Simple Problem of Resonant Scattering

In the present section, we restrict ourselves to one of the simplest models that causes resonant scattering, namely scattering due to a square-well potential. This model is also one of the rare solvable examples without the help of the imaginary gauge transformation, which we will formulate in the next section.

## 3.1 Square-Well Potential

We consider a finite potential well given by (Fig. 1)
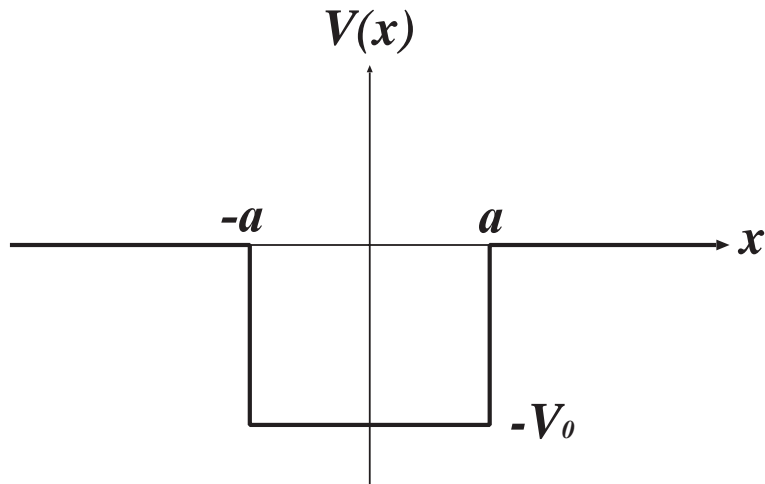


Figure 1: The square-well potential.

$$V(x) = \begin{cases} 0 & (x < -a), \\ -V_0 & (-a < x < a), \\ 0 & (a < x), \end{cases} \tag{3.1}$$

with $V_0 > 0$. In this model, transmission resonance occurs when the incident energy is equal to

$$E_{res} = -V_0 + \frac{n^2 \pi^2 \hbar^2}{8ma^2} \qquad (n = 1, 2, 3, \cdots), \tag{3.2}$$

as long as Eq (3.2) has a positive value.

In the following, we solve the Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \tag{3.3}$$

with the potential (3.1) under the boundary condition (2.9), which allows resonant states. In fact, we can obtain not only the resonant states but also the bound states. As usual, we introduce the parameters

$$k^2 = \frac{2mE}{\hbar^2}, \tag{3.4}$$

and

$$\kappa^2 = \frac{2m(E + V_0)}{\hbar^2}. \tag{3.5}$$

However, both $k$ and $\kappa$ are complex in general, since we wish to obtain the resonant states, which are characterized by complex energy eigenvalues $E$. Hence we write

$$k = k_r - i\gamma, \tag{3.6}$$
$$\kappa = \kappa_r - i\lambda, \tag{3.7}$$

where $k_r$, $\gamma$, $\kappa$ and $\lambda$ are real.

Using these parameters, we can write down the solution in each region of the potential (3.1) immediately as follows:

$$\psi(x) = \begin{cases} Ae^{-ikx} & (x < -a), \\ Be^{i\kappa x} + Ce^{-i\kappa x} & (-a < x < a), \\ De^{ikx} & (a < x), \end{cases} \tag{3.8}$$

where $A$, $B$, $C$ and $D$ are in general complex coefficients. Then we require the conditions that the wave functions and its first derivatives are continuous at $x = \pm a$. Because of the symmetry $V(-x) = V(x)$, we expect solutions of a definite parity. Therefore it is sufficient to apply the matching conditions to the solutions and its derivatives only at $x = a$. Thus we obtain

$$De^{ika} = Be^{i\kappa a} + Ce^{-i\kappa a}, \tag{3.9}$$

$$ikDe^{ika} = i\kappa Be^{i\kappa a} - i\kappa Ce^{-i\kappa a}. \tag{3.10}$$

Now let us examine even solutions and odd solutions separately.

**Even solutions:** In this case, we can set $A = D$ and $B = C$. Thus we rewrite Eqs. (3.9) and (3.10) as follows:

$$\alpha e^{ika} = 2\cos(\kappa a), \tag{3.11}$$

$$ik\alpha e^{ika} = -2\kappa \sin(\kappa a), \tag{3.12}$$

where $\alpha = A/B$. From the above equations, we obtain

$$ik = -\kappa \tan(\kappa a). \tag{3.13}$$

On the other hand, we obtain from (3.4) and (3.5), the relation

$$\kappa^2 - k^2 = \frac{2mV_0}{\hbar^2}. \tag{3.14}$$

Let us introduce the dimensionless parameters

$$\xi = ka, \tag{3.15}$$
$$\eta = \kappa a. \tag{3.16}$$

Using these parameters, Eqs. (3.13) and (3.14) can be rewritten in the form:

$$i\xi = -\eta \tan \eta, \tag{3.17}$$

$$\eta^2 - \xi^2 = \rho^2, \tag{3.18}$$

where

$$\rho^2 = \frac{2mV_0 a^2}{\hbar^2}. \tag{3.19}$$

Eliminating the variable $\xi$, we obtain

$$\eta = \pm\rho \cos \eta. \tag{3.20}$$

Now let us write the complex variable $\eta$ explicitly as

$$\eta = \mu - i\nu, \tag{3.21}$$

where

$$\mu = a\kappa_r, \tag{3.22}$$
$$\nu = a\lambda. \tag{3.23}$$

Equating the real parts and the imaginary parts of the both sides of Eq. (3.20) respectively, we obtain a set of simultaneous equations

$$\mu = \pm\rho\cos\mu\cosh\nu, \tag{3.24}$$
$$\nu = \mp\rho\sin\mu\sinh\nu. \tag{3.25}$$

Although we cannot proceed to solve this equation analytically any longer, the desired energy eigenvalues can be obtained numerically. If we plot the function

$$\nu = \cosh^{-1}\left(\frac{\mu}{\pm\rho\cos\mu}\right), \tag{3.26}$$

and Eq. (3.25) as functions of $\mu$, the intersections of these curves (Fig. 2) determine the eigenvalues from (3.5) as

$$E = -V_0 + \frac{V_0}{\rho^2}(\mu - i\nu)^2, \tag{3.27}$$

for a given $\rho$. Thus Eq. (3.27) yields the resonant level and the inverse lifetime respectively:

$$E_r = -V_0 + \frac{V_0}{\rho^2}(\mu^2 - \nu^2), \tag{3.28}$$
$$\Gamma = \frac{4V_0\mu\nu}{\rho^2}. \tag{3.29}$$

To obtain the wave functions for $x > |a|$, we must also determine the complex wave number $k$. From Eq. (3.17), we can calculate $k_r$ and $\gamma$ as follows:

$$ak_r = \frac{\nu\sin(2\mu) + \mu\sinh(2\nu)}{\cos(2\mu) + \cosh(2\nu)}, \tag{3.30}$$

$$a\gamma = \frac{\nu\sinh(2\nu) - \mu\sin(2\mu)}{\cos(2\mu) + \cosh(2\nu)}. \tag{3.31}$$

For simplicity of the calculation, we write, using Eq. (3.11),

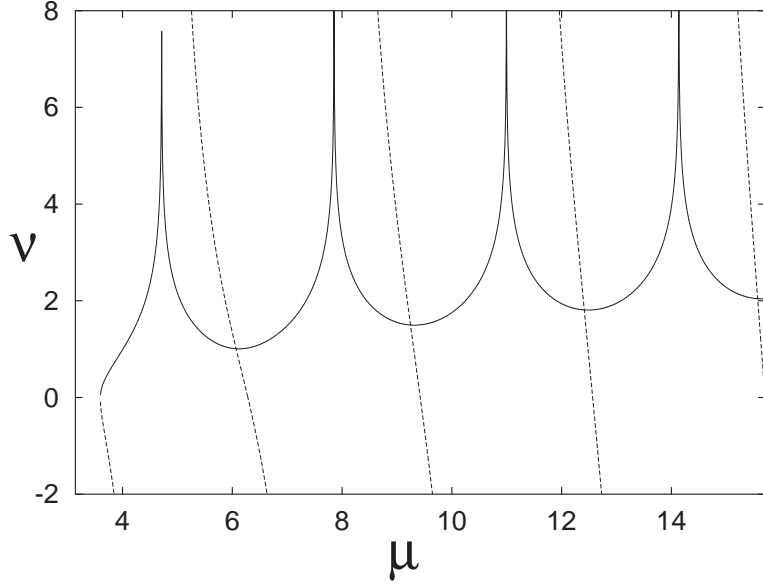$$A = 2\cos(\kappa a), \tag{3.32}$$
$$B = e^{ika}. \tag{3.33}$$

10

Figure 2: Equations (3.24) and (3.25). The intersections indicate the location of discrete complex eigenvalues for even solutions in squre well ($\rho = 4$ and $\pi \leq \mu \leq 5\pi$).

Thus the even wave function in the region of $x > a$, $\psi(x) = Ae^{ikx}$, is written in the form

$$
\begin{aligned}
\mathrm{Re}\psi(x) &= 2[\cos(\kappa_r a)\cosh(\lambda a)\cos(k_r x) \\
&\quad - \sin(\kappa_r a)\sinh(\lambda a)\sin(k_r x)]e^{\gamma x},
\end{aligned}
\tag{3.34}
$$

$$
\begin{aligned}
\mathrm{Im}\psi(x) &= 2[\cos(\kappa_r a)\cosh(\lambda a)\sin(k_r x) \\
&\quad + \sin(\kappa_r a)\sinh(\lambda a)\cos(k_r x)]e^{\gamma x}.
\end{aligned}
\tag{3.35}
$$

whereas in the region of $x < |a|$, the wave function $\psi(x) = 2B\cos(\kappa x)$ can be written as follows:

$$
\begin{aligned}
\mathrm{Re}\psi(x) &= 2e^{\gamma a}[\cos(k_r a)\cos(\kappa_r x)\cosh(\lambda x) \\
&\quad - \sin(k_r a)\sin(\kappa_r x)\sinh(\lambda x)],
\end{aligned}
\tag{3.36}
$$

$$
\begin{aligned}
\mathrm{Im}\psi(x) &= 2e^{\gamma a}[\cos(k_r a)\sin(\kappa_r x)\sinh(\lambda x) \\
&\quad + \sin(k_r a)\cos(\kappa_r x)\cosh(\lambda x)].
\end{aligned}
\tag{3.37}
$$

11

**Odd solutions:** We can also obtain the odd solutions by following the same procedure for calculating the even solutions except for setting $A = -D$ and $B = -C$. In this case, Eqs. (3.9) and (3.10) are written in the form

$$-\alpha e^{ika} = 2i\sin(\kappa a), \tag{3.38}$$

$$-k\alpha e^{ika} = 2\kappa\cos(\kappa a). \tag{3.39}$$

Thus Eq. (3.17) is changed into

$$i\xi = \eta\cot\eta. \tag{3.40}$$

Substituting this equation in the relation (3.18) yields

$$\eta = \pm\rho\sin\eta. \tag{3.41}$$

The simultaneous equations corresponding to Eqs. (3.24) and (3.25) are obtained as follows:

$$\mu = \pm\rho\sin\mu\cosh\nu, \tag{3.42}$$
$$\nu = \pm\rho\cos\mu\sinh\nu. \tag{3.43}$$

Once we know the solutions of the above equations numerically (Fig. 3), from Eq. (3.40), we can determine $k_r$ and $\gamma$ as

$$ak_r = \frac{\mu\sinh(2\nu) - \nu\sin(2\mu)}{\cosh(2\nu) - \cos(2\mu)}, \tag{3.44}$$

$$a\gamma = \frac{\nu\sinh(2\nu) + \mu\sin(2\mu)}{\cosh(2\nu) - \cos(2\mu)}. \tag{3.45}$$

As we mentioned above, the energy eigenvalues are given by Eq. (3.27). Furthermore, the wave functions can be obtained from Eq. (3.38) by setting

$$A = -2i\sin(\kappa a), \tag{3.46}$$
$$B = e^{ika}. \tag{3.47}$$

The odd solution for $x > a$ is given by

$$\begin{aligned}
\text{Re}\psi(x) = \ &2[\cos(\kappa_r a)\sinh(\lambda a)\cos(k_r x) \\
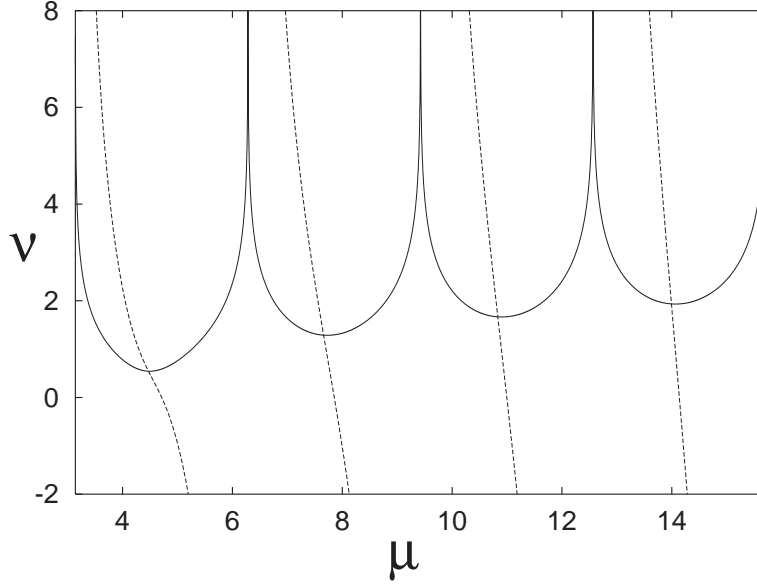&- \sin(\kappa_r a)\cosh(\lambda a)\sin(k_r x)]e^{\gamma x}, \tag{3.48}
\end{aligned}$$

12

Figure 3: Equations (3.42) and (3.43). The intersections indicate the location of discrete complex eigenvalues for odd solutions in squre well ($\rho = 4$ and $\pi \le \mu \le 5\pi$).

$$\text{Im}\psi(x) = 2[\cos(\kappa_r a)\sinh(\lambda a)\sin(k_r x) \\ + \sin(\kappa_r a)\cosh(\lambda a)\cos(k_r x)]e^{\gamma x}. \qquad (3.49)$$

On the other hand, the solution for $x < |a|$, $\psi(x) = 2iB\sin(\kappa x)$, is written in the form

$$\text{Re}\psi(x) = 2e^{\gamma a}[\cos(k_r a)\cos(\kappa_r x)\sinh(\lambda x) \\ - \sin(k_r a)\sin(\kappa_r x)\cosh(\lambda x)], \qquad (3.50)$$

$$\text{Im}\psi(x) = 2e^{\gamma a}[\cos(k_r a)\sin(\kappa_r x)\cosh(\lambda x) \\ + \sin(k_r a)\cos(\kappa_r x)\sinh(\lambda x)]. \qquad (3.51)$$

## 3.2 Numerical Results

Choosing the unit of $\hbar^2/2m = 1$, we obtained the resonance solutions numerically for the special case $\rho = 4$, $V_0 = 4$ and $a = 2$. The results of the

13

first eight solutions are summarized in Table 1. The agreement between the estimates $|E|$ and the theoretical value (3.2) of the resonant level $E_{res}$ is fairly good, although there seems to be no simple reason why it should be so. The divergent wave functions are also exemplified in Fig. 4.

| $n$ | $E_{res}$ | $E_r$ | $\Gamma/2$ | $\Gamma^{-1}$ | $|E|$ |
|---|---|---|---|---|---|
| 3 | 1.5517 | 0.9259 | 1.2142 | 0.41179 | 1.5269 |
| 4 | 5.8696 | 4.9552 | 3.0594 | 0.16343 | 5.8236 |
| 5 | 11.4213 | 10.2560 | 4.9354 | 0.10131 | 11.3817 |
| 6 | 18.2066 | 16.8183 | 6.9276 | 0.072175 | 18.1892 |
| 7 | 26.2257 | 24.6361 | 9.0328 | 0.055354 | 26.2398 |
| 8 | 35.4784 | 33.7049 | 11.2404 | 0.044482 | 35.5298 |
| 9 | 45.9649 | 44.0217 | 13.5401 | 0.036927 | 46.0570 |
| 10 | 57.6850 | 55.5842 | 15.9228 | 0.031402 | 57.8199 |

Table 1: Results of the square-well potential. Theoretical values $E_{res}$ are obtained from Eq. (3.2).
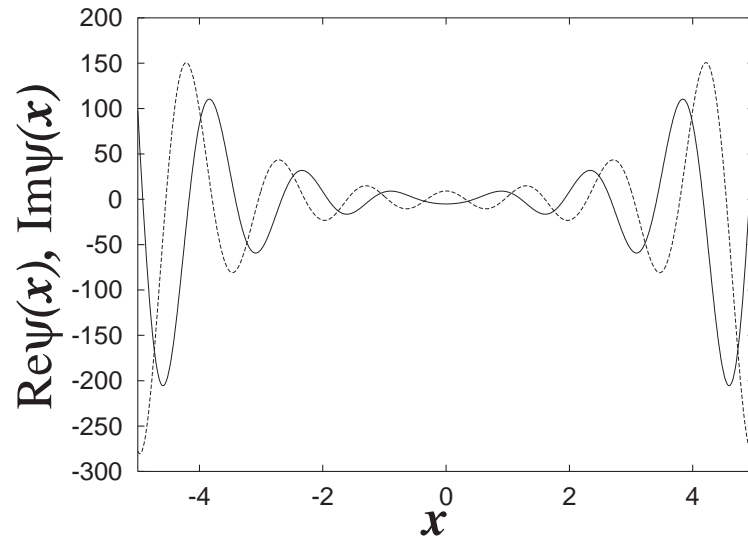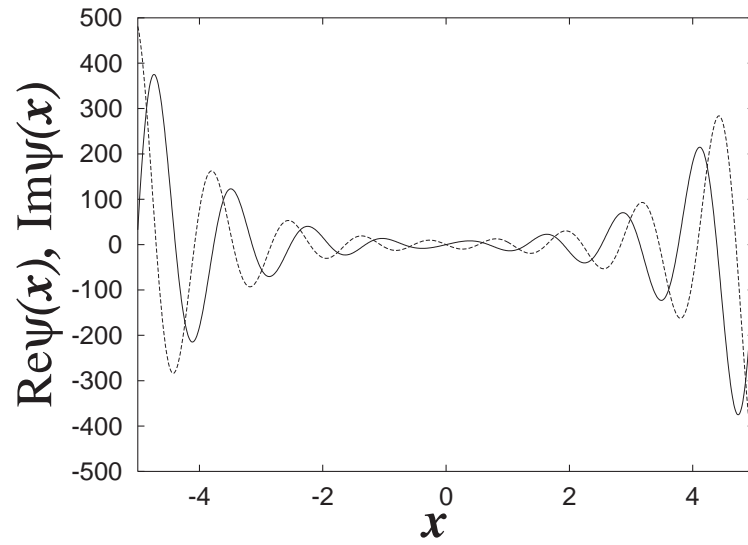
Figure 4: The resonant wave functions. The solid line and the broken line indicate the real part and the imaginary part of the solution respectively. (a) Even solutions with the eigenvalue $E = 16.8183 - i6.9276$. (b) Odd solutions with $E = 24.6361 - i9.0328$.

# 4 Imaginary Gauge Transformation

In the present section, the general formulation of the imaginary gauge transformation is proposed. By means of this transformation, the usual Hamiltonians are converted to non-Hermitian operators. We can thereby expand the region of the convergent solutions.

## 4.1 The General Formulation

First, we consider the standard one-body Hermitian Hamiltonian in the $d$-dimensional continuum space,

$$\mathcal{H}_0 = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}), \tag{4.1}$$

where $\mathbf{p} = (\hbar/i)\nabla$ is the momentum operator and $V(\mathbf{x})$ is a potential. What to obtain are the eigenfunctions of the resonant states of the Schrödinger equation

$$\mathcal{H}_0\psi_0(\mathbf{x}) = E_0\psi_0(\mathbf{x}), \tag{4.2}$$

where $\psi_0(\mathbf{x})$ is a diverging wave function as $|\mathbf{x}| \to \infty$ and $E_0$ is a complex energy eigenvalues. For this purpose, we treat the non-Hermitian Hamiltonian of the form

$$\mathcal{H}_g = \frac{(\mathbf{p} + i\mathbf{g}(\mathbf{x}))^2}{2m} + V(\mathbf{x}) \tag{4.3}$$

instead of $\mathcal{H}_0$. Here $\mathbf{g}(\mathbf{x})$ is a spatially varying real vector referred to as the imaginary vector potential. The Hamiltonian (4.3) can be written more explicitly as

$$\mathcal{H}_g = -\frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar}{m}\mathbf{g}(\mathbf{x})\cdot\nabla + \frac{\hbar}{2m}\nabla\cdot\mathbf{g}(\mathbf{x}) - \frac{\mathbf{g}(\mathbf{x})^2}{2m} + V(\mathbf{x}). \tag{4.4}$$

Of course, in the case $\mathbf{g}(\mathbf{x}) = \mathbf{0}$, Eqs. (4.3) and (4.4) are reduced to the standard Hamiltonian (4.1).

The eigenfunction of the Hamiltonian $\mathcal{H}_g$ corresponding to $\psi_0(\mathbf{x})$ is given by the gauge-transformed function

$$\psi_g(\mathbf{x}) = \exp\left[\frac{1}{\hbar}\int^{\mathbf{x}}\mathbf{g}(\mathbf{x}')\cdot d\mathbf{x}'\right]\psi_0(\mathbf{x}). \tag{4.5}$$

On the other hand, the eigenvalue $E_0$ must remain the same as long as $\mathbf{g}(\mathbf{x})$ can be expressed as the gradient of an arbitrary scalar function. The readers can confirm

$$\mathcal{H}_g \psi_g(x) = E_0 \psi_g(x) \tag{4.6}$$

by plugging (4.5) into (4.6) and making straightforward algebra. From now on, we write the energy eigenvalue simply as $E$ instead of $E_0$.

Consequently, choosing an appropriate gauge $\mathbf{g}(\mathbf{x})$, we can obtain $\psi_g(\mathbf{x})$ as a bound state with the complex eigenvalue $E$ even if $\psi_0(\mathbf{x})$ is a diverging function. In other words, the problem of obtaining the resonant state is reduced to the bound-state problem.

## 4.2  The One-Dimensional System

In the following, we focus on the one-dimensional case. Equation (4.3) is reduced to the Hamiltonian

$$\mathcal{H}_g = \frac{(p + ig(x))^2}{2m} + V(x), \tag{4.7}$$

where $p = (\hbar/i)d/dx$. The Schrödinger equation (4.4) is written in the form

$$\left[ \frac{d^2}{dx^2} - \frac{1}{\hbar}\frac{d}{dx}g(x) - \frac{g(x)}{\hbar}\frac{d}{dx} + \frac{g(x)^2}{\hbar^2} - \frac{2m}{\hbar^2}(V(x) - E) \right] \psi_g(x) = 0. \tag{4.8}$$

Here we note that

$$\frac{d}{dx}g(x) = g'(x) + g(x)\frac{d}{dx}, \tag{4.9}$$

Thus we can rewite Eq. (4.8) as follows:

$$\left[ \frac{d^2}{dx^2} - \frac{2g(x)}{\hbar}\frac{d}{dx} - \frac{g'(x)}{\hbar} + \frac{g(x)^2}{\hbar^2} - \frac{2m}{\hbar^2}(V(x) - E) \right] \psi_g(x) = 0. \tag{4.10}$$

**Choice of the gauge:** Now we must determine the imaginary vector potential $g(x)$ concretely. Assuming that the wave function of resonant states has an asymptotic form $\psi_0(x) \sim e^{ik_r|x|+\gamma|x|}$, the gauge factor $\exp[\frac{1}{\hbar}\int^x g(x')dx']$ should behave as $e^{-c|x|}$ as $|x| \to \infty$. For this reason, we choose the gauge as follows:

$$g(x) = -g_0 \tanh\left(\frac{g_0 x}{\hbar}\right), \tag{4.11}$$

18

where $g_0$ is a positive constant, which determines the strength of the suppression of the divergence of the wave function. In this case, Eq. (4.5) gives the eigenfunction of the Schrödinger equation $\mathcal{H}_g \psi_g(x) = E\psi_g(x)$ in the form

$$\psi_g(x) = \frac{1}{\cosh(g_0 x/\hbar)}\psi_0(x). \tag{4.12}$$

This gauge-transformed solution $\psi_g(x) \sim e^{ik_r|x|-(g_0-\gamma)|x|}$ is convergent for $g_0 > \gamma$ and thus can be handled easily. The Hamiltonian $\mathcal{H}_g$ in Eq. (4.10) takes the form

$$\mathcal{H}_g = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{\hbar}{m}g_0 \tanh\left(\frac{g_0 x}{\hbar}\right)\frac{d}{dx} - \frac{g_0^2}{2m} + V(x). \tag{4.13}$$

We treat this non-Hermitian Hamiltonian for a practical problem in the next section.

# 5 Numerical Analysis

The methodology formulated in the previous section can be applicable to extensive problems. Its application to a one-dimensional problem and all the numerical results obtained are described in the present section.

## 5.1 Matrix Representation of the Hamiltonian

The problem to be solved is the Schrödinger equation

$$\tilde{\mathcal{H}}_g \psi_g(x) = \tilde{E}\psi_g(x), \tag{5.1}$$

where

$$\tilde{\mathcal{H}}_g = -\frac{d^2}{dx^2} - \frac{2g_0}{\hbar}\tanh\left(\frac{g_0 x}{\hbar}\right)\frac{d}{dx} - \frac{g_0^2}{\hbar^2} + \tilde{V}(x), \tag{5.2}$$

and

$$\tilde{V}(x) = \frac{2m}{\hbar^2}V(x), \tag{5.3}$$

$$\tilde{E} = \frac{2m}{\hbar^2}E, \tag{5.4}$$

for a given $V(x)$ under the boundary conditon that is the same as bound states. This is essentially a bound-state problem except that the Hamiltonian is not Hermitian.
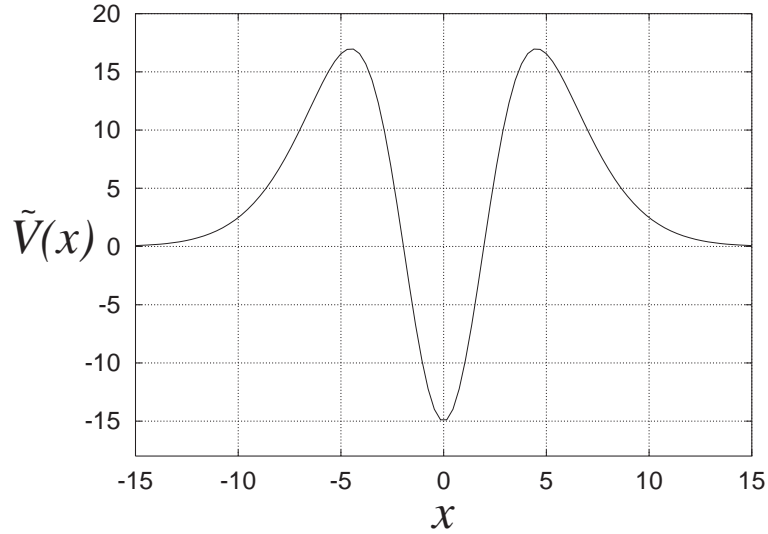
19

Figure 5: The potential (5.5) (A combination of two Gaussian functions).

We assume that the usual method of solving the bound-state problem is still valid for this non-Hermitian case. Here we express the eigenfunctions as a superposition of an appropriate function system. The merit of this method is that the resonant energy and the lifetime can be obtained directly as complex eigenvalues of the Hamiltonian matrix.

Now we consider the potential which is a combination of two Gaussian functions (Fig. 5)

$$\tilde{V}(x) = 5(8e^{-(x/6)^2} - 11e^{-(x/3)^2}). \tag{5.5}$$

In terms of the eigenfunctions of the harmonic oscillator $\varphi_n(x)$, we expand $\psi_g(x)$ as

$$\psi_g(x) = \sum_{n=0}^{\infty} c_n \varphi_n(x), \tag{5.6}$$

where $c_n$ is the expansion coefficient. The complete orthonormal set $\{\varphi_n(x)\}$ which satisfies

$$\left( -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2 \right) \varphi_n(x) = E\varphi_n(x), \tag{5.7}$$

20

is given by

$$\varphi_n(x) = \frac{1}{\sqrt{\beta\sqrt{\pi}2^n n!}} H_n(\xi)e^{-\xi^2/2} \qquad (n = 0, 1, 2, \cdots), \qquad (5.8)$$

where

$$\beta = \sqrt{\frac{\hbar}{m\omega}}, \qquad (5.9)$$

$$\xi = \frac{x}{\beta}, \qquad (5.10)$$

and $H_n(\xi)$ is the Hermite polynomials. Adopting the Dirac bra-ket notation, we obtain the matrix elements of $\tilde{\mathcal{H}}_g$ as

$$(\tilde{\mathcal{H}}_g)_{ij} = \langle\varphi_i|\tilde{\mathcal{H}}_g|\varphi_j\rangle. \qquad (5.11)$$

In practice, the expansion (5.6) must be truncated at a finite number of basis in order to diagonalize the matrix (5.11) numerically.

On the basis of the argument in Sec. 4, the non-Hermitian matrix (5.11) may have resonant states as complex eigenvalues which are independent of $g_0$. Once we find such solutions, we obtain the divergent wave functions $\psi_0(x)$ from Eq. (4.12) by gauge-transforming back from $\psi_g(x)$.

The resonant levels are approximately equal to the levels that would be bound states if the potential barriers are infinitely high. Thus we can roughly estimate the locations of the resonant states by approximating (5.5) in the form $\tilde{V}(x) \simeq 5x^2 - 15$. Therefore we expect that there are at least four long-lived resonant states at

$$\tilde{E}_{res} \simeq 5.1, \ 9.6, \ 14.1, \ 18.5 \qquad (5.12)$$

and four bound states at

$$\tilde{E}_b \simeq -12.8, \ -8.3, \ -3.8, \ \ 0. \qquad (5.13)$$

## 5.2 Results and Discussions

We present the eigenvalue spectrum of the non-Hermitian matrix (5.11) with $g_0 = 0.0$, 0.6 and 0.8 in Fig. 6. The discrete eigenvalues independent of $g_0$ on the negative real axis correspond to bound states. There are four energy

levels of the bound states at $\tilde{E}_b = -12.8129, -8.5400, -4.4743, -0.6262$, which are consistent with (5.13).

The spectrum shows two resonant states at $\tilde{E} \simeq 15.2 - i2.3,\ 18.9 - i3.1$, which are in fairly good agreement with the expected values (5.12). We exemplify the corresponding eigenfunction $\psi_g(x)$ and the divergent wave function $\psi_0(x)$ in Fig. 7.

The eigenvalues located in the positive real axis at $\tilde{E}_r \simeq 6.3,\ 9.4$ presumably correspond to the other two expected resonant levels. We expect that these two eigenvalues become complex when we increase the dimensions of the matrix (5.11).
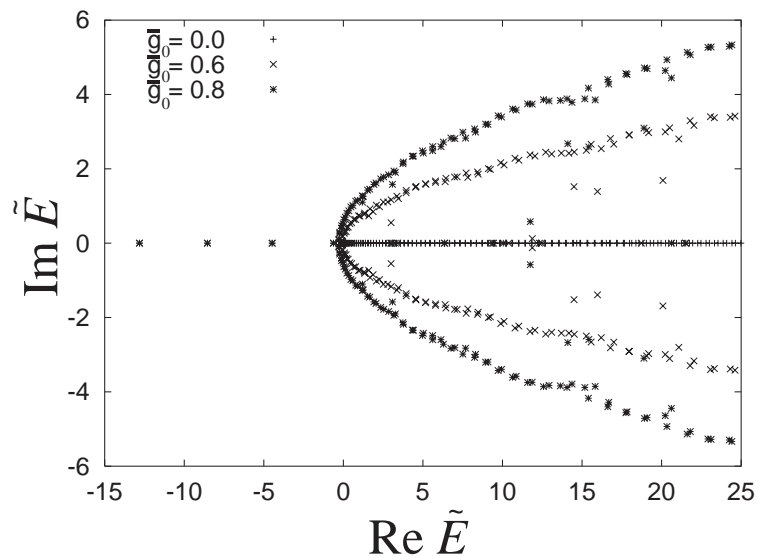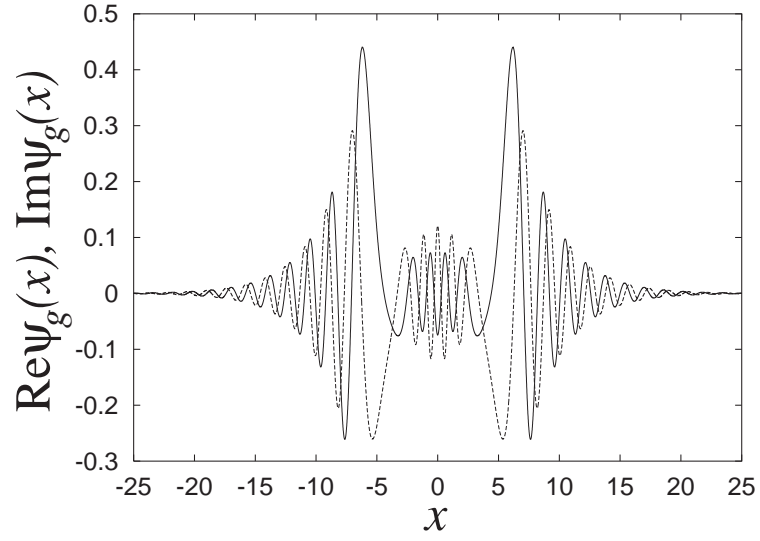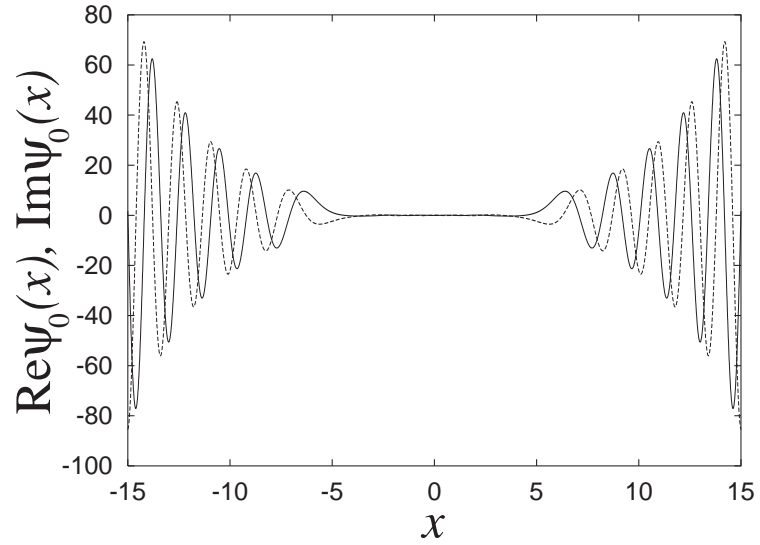


Figure 6: The energy spectrum of the non-Hermitian model (5.2) with dimensions 400 and $\beta = 2$. $(\bar{g}_0 = g_0/\hbar)$.

(a)



(b)

Figure 7: The convergent and divergent eigenfunctions. The solid line and the broken line indicate the real part and the imaginary part of the solution respectively. (a) The gauge-transformed convergent eigenfunction $\psi_g(x)$ with $g_0 = 0.6$. (b) The divergent wave function of the resonant state $\psi_0(x)$ with $\tilde{E} = 15.2 - i2.3$.

# 6 Conclusion

We investigated resonant states numerically in the framework of non-Hermitian quantum mechanics. In Sec. 3, we obtained the divergent wave functions corresponding to the resonant states under the boundary conditions for the open quantum system as we explained in Sec. 2. The modulus of the obtained eigenvalues is in good agreement with the theoretically predicted values. In Sec. 4, We introduced the imaginary vector potential in order to expand the region of the convergent solutions of the Schrödinger equation. In Sec. 5, we found resonant levels and their lifetimes directly as complex eigenvalues of a non-Hermitian matrix. We confirmed that the divergent wave function of the resonant states can be obtained as a gauge-transformed convergent eigenfunction with the complex eigenvalues. We showed that the imaginary gauge transformation is a convenient way of defining resonant states as well as computing them.

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## References

[1] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).

[2] Y. Imry, *Introduction to Mesoscopic Physics* (Oxford University Press, New York, 1997).

[3] K. Na and L. E. Reichl, Phys. Rev. B **59**, 13 073 (1999).

[4] D. Boese, M. Lischka and L. E. Reichl, Phys. Rev. B **61**, 5632 (2000).

[5] J. Aguilar and J. M. Combes, Commun. Math. Phys. **22**, 269 (1971).

[6] E. Balslev and Combes, Commun. Math. Phys. **22**, 280 (1971).

[7] N. Hatano and D. R. Nelson, Phys. Rev. Lett. **77**, 570 (1996).

[8] N. Hatano and D. R. Nelson, Phys. Rev. B **56**, 8651 (1997).

[9] N. Hatano and D. R. Nelson, Phys. Rev. B **58**, 8384 (1998).

[10] N. Hatano, Physica A **254**, 317 (1998).

[11] N. Hatano, T. Watanabe and J. Yamasaki, (to be published).