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Schrödinger equation with imaginary potential

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Abstract

We numerically investigate the solution of the Schrödinger equation in a one-dimensional system with gain. The gain is introduced by adding a positive imaginary potential in the system. We find that the time-independent solution gives that the amplification suppresses wave transmission at large gain. Solutions from the time-dependent equation clearly demonstrate that when gain is above a threshold value, the amplitude of the transmitted wave increases exponentially with time. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Transfer matrix; Gain; Disorder; Non-hermitian systems

1. Introduction

Recently the propagation of classical wave in gain media has been studied [1–10]. With enhanced optical paths from multiple scattering, one would expect the transmission coefficient in disordered systems to be also enhanced with gain. Surprisingly transfer matrix calculation [1,2] based on time-independent wave equations showed that for large systems the wave propagation is suppressed with gain, leading to smaller transmission [3,4] of waves as if the system was absorbing. Thus, it was generally believed that the paradoxical phenomenon may indicate enhanced localization due to interference of coherently amplified multiple reflected waves [1–8]. To fully understand the origin of this apparent non-intuitive suppression of transmission, Jiang et al. [10] examined the validity of the solutions derived from the time-independent wave equations which have been commonly employed in describing the wave propagation in active media. Linearized time-independent wave equations with complex dielectric constant have been successfully applied to find lasing modes by locating the poles in the complex frequency plane [11] and to investigate the spontaneous emission noise below the lasing threshold in distributed feedback semiconductor lasers [12]. Nevertheless, these successes cannot be extended in general to actual lasing phenomena since a steady output assumption may lead to unphysical solution. Jiang et al. pointed out that any preassumed time-independent wave solutions are insufficient to interpret wave propagation in gain media. When the gain is large enough or the system is long enough to exceed the critical value, the time-independent solution even gives a wrong picture. They also emphasized that the apparent suppression is not due to the disorder or other forms of localization. With sufficient gain, wave should be able to overcome losses from backscattering and propagate through the system with increased intensity.

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In this paper we want to check whether a similar behavior can be seen in a quantum system. We study the solution of the Schrödinger equation with a complex potential as a mathematical model. We interpret the positive imaginary potential as gain since the probability density of the system is increasing with time. By solving the time-independent Schrödinger equation we indeed find that the transmission coefficient decreases even in the presence of gain. The numerical simulations show that the probability density has the same behavior as the classical EM wave.

Section 2 describes our model. We introduce the gain by adding a positive constant imaginary potential to the Schrödinger equation. Section 3 gives a summary of our simulation results. It shows how the time-independent solution is broken down. Section 4 is conclusion.

2. Model

In a one-dimensional system with complex square well potential, the time-dependent Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,t), \tag{1}$$

where $V(x) = 0$ for $x < 0$ or $x > L$ and $V(x) = -V_0 + \mathrm{i}V_\mathrm{I}$ otherwise, where $V_0 > 0$.

For a time-independent solution, the above equation is equivalent to time-independent Maxwell wave equation

$$\frac{\partial^2 E(x)}{\partial x^2} + \frac{\omega^2}{c^2}\varepsilon(x)E(x) = 0 \tag{2}$$

with $\varepsilon = \varepsilon_0 + \varepsilon_\mathrm{I}$, ε_I is defined in between 0 and L.

Note the Hamiltonian in our Schrödinger equation is non-Hermitian, the wave function cannot be normalized and the probability is not a local variable, therefore $(\mathrm{d}/\mathrm{d}t)\int_{-\infty}^{\infty}|\psi(x,t)|^2\,\mathrm{d}^3x \neq 0$. There are a couple of papers which are dealing with non-Hermitian Quantum Mechanics [13,14], but for the time being we just perform numerical simulation for time-dependent solution on our model. We use a well-developed finite difference time domain (FDTD) technique [15] to simulate the time evolution for the Schrödinger equation. The evolution of the wave function at a later time is expressed by

$$\psi^{n+1} = \mathrm{e}^{-\mathrm{i}(H/\hbar)\Delta t}\psi^n. \tag{3}$$

We use the following approximation to compute the evolution operator [16]:

$$\mathrm{e}^{-\mathrm{i}(H/\hbar)\Delta t} \simeq \frac{1 - \mathrm{i}H\Delta t/2\hbar}{1 + \mathrm{i}H\Delta t/2\hbar}. \tag{4}$$

In Hermitian case, i.e. if $V_\mathrm{I} = 0$, the norm of the right-hand side expression is 1, thus it is a good approximation since it can automatically satisfy both the stability requirement imposed on discretion and wave function and normalization of the wave function. Later in our numerical calculation, the V_I is some non-zero values due to the introduction of the gain. The wave source we used in our simulation is

$$\varphi_{\mathrm{src}}(t) = \begin{cases} \mathrm{e}^{-(t-t_0)^2/t_1^2}\mathrm{e}^{-\mathrm{i}\omega t}, & t \leqslant t_0, \\ \mathrm{e}^{-\mathrm{i}\omega t}, & t > t_0, \end{cases} \tag{5}$$

where t_0 and t_1 are two constants which define a gradually increased modulation on wave form. t_0 indicates the moment when the wave source begins to give off steady output. t_1 indicates the width of modulation, so it defines how smooth the modulation is. The reason to add a gradually increased modulating factor is to allow a smooth transition to the steady state and to maintain the stability of the simulation.

In our computation, a complex potential with a width $L = 0.2$ μm is used. Several positive imaginary potentials were chosen and the corresponding transmission coefficients were calculated. The Liao absorption boundary condition [15] at the far ends of the system leads was used to avoid mixing of the transmitted and reflected waves.

3. Results

First we present the time-independent numerical results. In Fig. 1 we plot the logarithm of the transmission coefficient versus the length L of the width of the complex potential. In this case $V_0 = 0.5411$ eV, $V_\mathrm{I} = 0.00449$ eV and the incident energy $E = 0.37628$ eV. Notice that the figure is

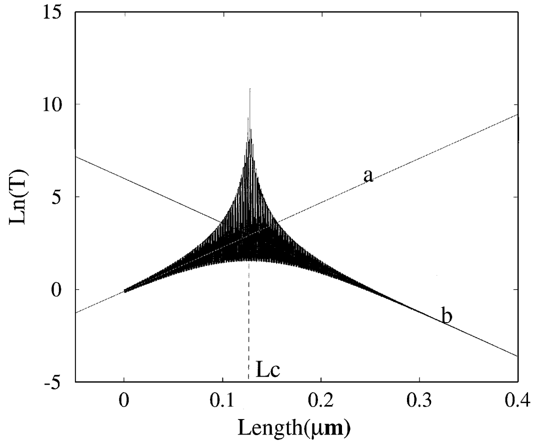

Fig. 1. Naïve time-independent solution for Schrödinger equation, $\ln(T)$ versus L. Note the drop if potential length is greater than L_c, which is unphysical. a and b are two asymptotic lines in the two limitation directions. (a) $L \to -\infty$, (b) $L \to +\infty$. The parameters used, $V_0 = 0.5441$ eV, $V_I = 0.00449$ eV, incident energy $E = 0.37628$ eV.

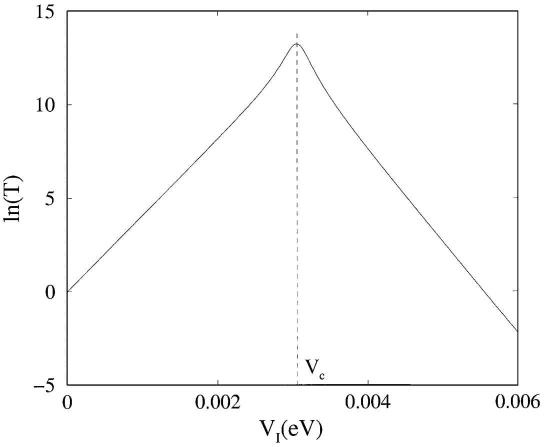

Fig. 2. Another view of the time-independent solution for Schrödinger equation, $\ln(T)$ versus gain V_I. This figure clearly shows the critical gain at a constant system length ($L = 0.2$ μm). Notice the unphysical drop after the critical gain V_I^c. The critical gain is defined as the extreme point in this graph.

exactly the same as that of Fig. 1 of Ref. [10]. In this electronic case too for large enough L, T drops despite the fact that we have gain. The solid lines in Fig. 1 give the asymptotic lines for $\ln(T)$ for positive and negative large L. For negative large L, $\ln(T) = 2k_1' L + l_2$, while for positive large L,

$$\ln(T) = -2k_1' L + l_1,$$

where

$$k_1' = \frac{1}{\hbar}\sqrt{m(E + V_0) + m\sqrt{(E + V_0)^2 + V_I^2}},$$

$$l_1 = \ln\left[16\Big/\left(\frac{k_1^2}{k^2}\left(1 + \frac{k}{k_1}\right)^4 + \frac{4k_1'^2}{k_1^2}\left(1 + \frac{k}{k_1}\right)^4\right)\right],$$

$$l_2 = \ln\left[16\Big/\left(\frac{k_1^2}{k^2}\left(1 - \frac{k}{k_1}\right)^4 + \frac{4k_1'^2}{k_1^2}\left(1 - \frac{k}{k_1}\right)^4\right)\right],$$

$$k = \sqrt{2mE/\hbar^2},$$

$$k_1 = mV_I/\hbar\sqrt{m(E + V_0) + m\sqrt{(E + V_0)^2 + V_I^2}}.$$

From the intersection of these two asymptotic lines we can evaluate the critical length $L_c(= \frac{1}{2}(l_1 + l_2))$, above which the time-independent solution is not valid.

In Fig. 2, we plot the logarithm of the transmission coefficient $\ln(T)$ versus the imaginary part of the potential V_I, for a constant width $L = 0.2$ μm of the complex potential. The critical value of the gain V_I^c is given to be approximately equal to 0.0032 eV. Notice again that for large V_I, $\ln(T)$ decrease despite the fact the gain (V_I) increases. We have again that gain effectively becomes loss at large gains. Remember, that the system is homogeneous, thus disorder is definitely not responsible for this strange behavior.

We can get a better understanding of how the wave function evolves inside the potential well, by analytically solving the time-dependent Schrödinger equation with a complex potential. The equation can be written as

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0\right)\psi(x,t) = \left(i\hbar\frac{\partial}{\partial t} - iV_I\right)\psi(x,t). \quad (6)$$

Separation of $\psi(x,t) = X(x)T(t)$ gives the following equation:

$$-\frac{\hbar^2}{2m}\frac{X''}{X} - V_0 = i\hbar\frac{T''}{T} - iV_I = E. \quad (7)$$

The solution of Eq. (7) suggests that the time dependency behaves as $[e^{V_I t/\hbar}]e^{-iEt/\hbar}$. The spatial part is a normal wave equation. In addition to the normalized factor $e^{-iEt/\hbar}$, we have an exponentially increased factor $e^{V_I t/\hbar}$, which cannot be captured by the time-independent equation. Ecomomou has pointed out that the time increase comes from the discrete spectra with imaginary energy eigenvalues [17]. The sum of all those discrete partial waves contribute the exponential time increase of the wave function.

The numerical solution of the time-dependent Schrödinger equation shows that below or above the critical gain the time-dependent behavior of wave function of each round trip inside the potential well are different. Below the critical gain, the increase of the wave function ψ after each round trip is getting smaller and smaller and eventually the output of the transmission can reach a steady-state solution. On the other hand, when the gain V_I is above the critical gain, the increase of ψ after each round trip is getting larger with time and causes ψ to have an exponential increase. This behavior is clearly seen in Fig. 3. Notice that for V_I larger than the critical gain, ψ increases exponentially with time. This is shown in Fig. 4, where the $\ln|\psi(t)|$ versus t is plotted for cases with gain both above and below the critical gain.

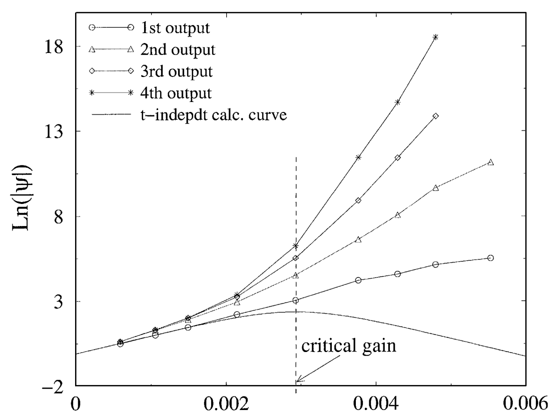

Fig. 3. Transmission versus V_I. The parameters we use are $L = 0.2$ μm, $V_0 = 0.5411$ eV. The "1st output" means the output of the first transmitted wave through the potential well. "2nd output" means the 2nd output, i.e. after the wave's first round trip inside the well (due to the reflection on potential boundaries), and so on. See the steps in curve a in Fig. 4.

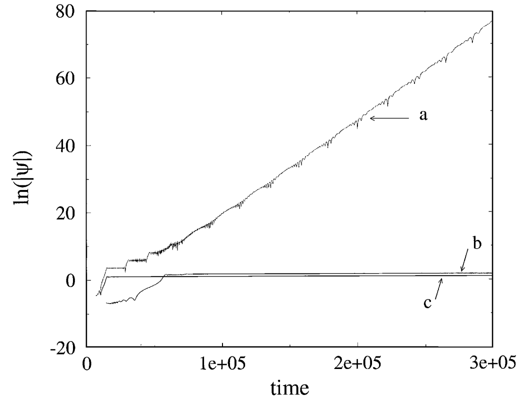

Fig. 4. Transmission versus time. The time step is 4.5×10^{-17} s. The parameters we use are: $L = 0.2$ μm, $V_0 = 0.5411$ eV, incident energy $E = 0.37642$. The critical gain $V_I^c \simeq 0.00292$ eV. The slope of the $\ln|\psi|$ versus t corresponding to $V_I/\hbar$. So we can have the value of V_I from the numerical simulation data. (a) Above the critical gain, $V_I = 0.004791$ eV, the calculated value of $V_I = 0.004703$ eV. (b) Below the critical gain, $V_I = 0.001055$ eV. The wave function reaches a steady value. (c) No gain, $V_I = 0$ eV.

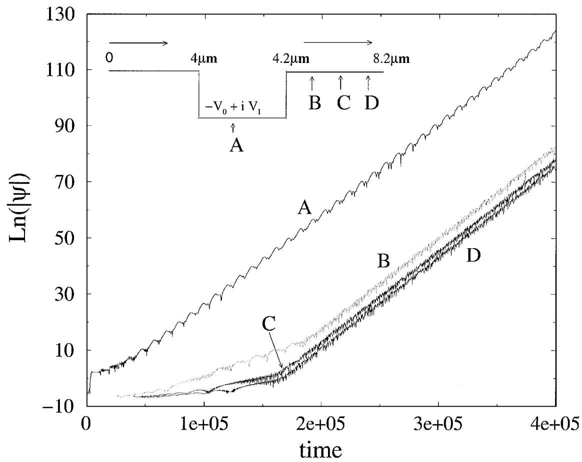

Fig. 5. Transmission versus time. The slope of the lines is approximately equal to $V_I/\hbar$ ($V_I = 0.004791$ eV versus $V_I^{\text{calculated}} = 0.004703$ eV), which implies that $\psi \propto e^{V_I t/\hbar}$ (inside and outside). The letters beside the lines correspond to the data collecting points shown above.

From Fig. 4 we have calculated the slope of the $\ln(|\psi|)$ with respect to time, and we found indeed that the transmitted wave function increases exponentially as $e^{V_I t/\hbar}$ when the gain is above the critical

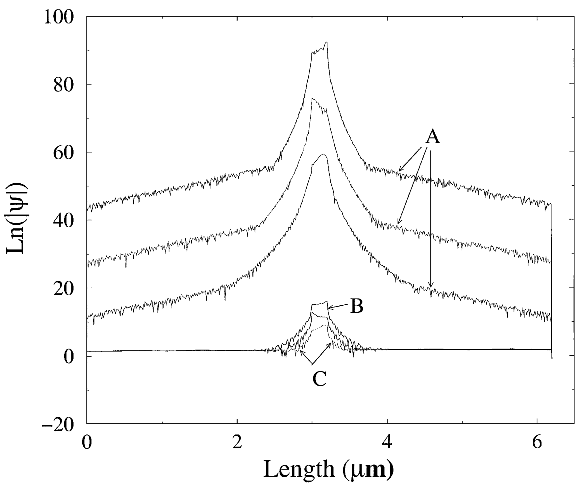

Fig. 6. Snapshots of the amplitude of the wave function for different V_I (at 3 time points. The time intervals are same between the points). The potential well is located at 3 μm ~ 3.2 μm. (A) Gain is above the critical value ($V_I = 0.004791$ eV). (B) Around the critical value ($V_I = 0.00292$ eV). (C) Below the critical value ($V_I = 0.001055$ eV).

value. When the gain is below the critical value, the transmitted wave reaches a constant value (see line b in Fig. 4). From Fig. 4, we can see the step-like behavior of the wave function, which indicates the different reflections at the boundaries of the complex potential function.

Our numerical results also shows that the wave function increases with time exponentially as $e^{V_I t/h}$ for both inside the potential well and outside the well. This is clearly shown in Fig. 5, where the $\ln(|\psi(t)|)$ versus t is plotted.

The overall distribution of the wave function along the system is also calculated. Fig. 6 shows if the gain is below the critical value, the output wave function is stable outside the potential well along the propagation direction. If the gain is above the critical value, the output wave function decreases exponentially outside the potential wall ($\propto e^{-\alpha x}$). The decrease is caused by the continuity condition of wave function on the complex potential boundary.

4. Conclusion

In summary, we have examined the solution of Schrödinger equation with gain. The computer simulation results are quite different from those obtained from time-independent equation using transfer matrix method. The difference is due to the wrong steady-output assumptions made by transfer matrix methods.

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