Constraints on the reciprocal propagation of a quantum particle through a 1D localized complex potential

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Abstract

In the propagation of an electron through a 1D asymmetric complex potential, it is known that while the conventional Green function reciprocity symmetry will ensure transmission to be symmetric between a "left-incident" and a "right-incident" beam, no such symmetry exists for the case of reflection. Here we derive generalized reciprocity relations for both the amplitude and phase of the reflected waves as constraints on the left and right incident beams, in complete analogy to what was established in optics. We further provide illustrations of these relations via direct analytical calculations in the case of a real potential, and via numerical studies in the case of a complex potential.

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PACS: 03.65.Nk

Introduction

The elementary problem of propagation of a quantum particle in a 1D potential is of fundamental interest from the beginning of quantum mechanics, with the prediction of the intriguing phenomenon of quantum tunneling which has found numerous applications in the literature [1]. Over the years, the study of this problem has been extended to potentials of various forms which can be complex [2, 3] and can serve as models for inelastic scattering with absorption of the particle to take place. For the general case when the potential is allowed to be asymmetric and complex, one interesting issue is about the possible reciprocal symmetry in the transmission and reflection of the particle with reference to a left-incident and a right-incident beam [4].

Consider an arbitrary potential as shown in Fig. 1. It is known that the transmission and reflection coefficients are identical whether the particle is incident from the left or from the right side in the case of real (non absorptive) potentials. In the case of a complex potential with absorption, one still has the same transmission for both the left- and right- incidence but the reflection coefficients will be in general different for particles incident from different sides of the potential [5, 6]. It thus appears that unless there is absorption, it is not possible to probe the asymmetry of a ***real*** potential via simple 1D scattering experiments by having different incident beams interacting with the potential [5, 7].

It is the purpose of our present work to point out that, by examining the various generalized reciprocity relations among the transmission and reflection waves, one can have both the transmitted and reflected waves related to each other in a definite way even in the presence of absorption, and that asymmetry can still be revealed in the case of real non-absorptive potentials. We shall first establish that, in complete analogy with the results established in optics, the two beams incident from opposite sides of the potential will have the same transmission amplitudes and phases, while those corresponding to the reflected beam will be different in general, except for the case of real potentials when the coefficient of reflection (amplitude modulus square) will be the same. We shall limit ourselves to localized potentials so that the incident particle with a real energy $(E > 0)$ will propagate as a free particle beyond a certain finite extent of spatial region.

Generalized Reciprocity Relations

In two studies on the reciprocity theorem in optics as applied to the propagation of light through a 1D stratified system composed of different materials, Agarwal and coworkers have derived certain generalized reciprocal relations between the reflected and transmitted light waves from identical beams incident from the two (left and right) sides of the medium [8, 9]. In particular, they have shown that while the transmitted fields are always identical from either side of the stratified system, the reflected fields will in general be different in both their amplitudes and phases. In the following, we shall first establish the analogous results for the matter waves in quantum mechanics, and shall then provide some illustrations from direct calculations of these waves.

Assuming the potential is localized within a region $x_1 \le x \le x_2$ with the potential $V = 0$ for $x < x_1$ and $x > x_2$, let us consider two electrons of wave functions ψ_1 and ψ_2 and identical energy E being incident from the left and right, respectively, as indicated as in Fig. 1 (a). The stationary Schrodinger equation and the asymptotic form for these waves (i.e. waves outside the potential zone) can thus be expressed as follows:

$$\frac{d^2\psi}{dx^2} + k^2\left(1 - \frac{V}{E}\right)\psi = 0, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \ , \qquad (1)$$

where

$$\psi_1 = \begin{cases} \psi_{1i} e^{ikx} + \psi_{1r} e^{-ikx} & \text{for} \quad x < x_1 \\ \psi_{1t} e^{ikx} & \text{for} \quad x > x_2 \end{cases} , \tag{2}$$

and

$$\psi_2 = \begin{cases} \psi_{2i} e^{-ikx} + \psi_{2r} e^{ikx} & \text{for} \quad x > x_2 \\ \psi_{2t} e^{-ikx} & \text{for} \quad x < x_1 \end{cases} . \tag{3}$$

Thus, applying (1) to ψ_1 and its conjugate to ψ_2, one can easily establish the following integral relations (for a complex potential):

$$\int_{-L}^{L} \left(\psi_2^* \frac{d^2\psi_1}{dx} - \psi_1 \frac{d^2\psi_2^*}{dx} \right) dx - \frac{k^2}{E} \int_{-L}^{L} \psi_1 \psi_2^* \left(V - V^* \right) dx = 0$$

$$\Rightarrow \qquad \int_{-L}^{L} \frac{d}{dx} \left(\psi_1 ' \psi_2^* - \psi_1 \psi_2^* ' \right) dx - \frac{k^2}{E} \int_{-L}^{L} \psi_1 \psi_2^* \left(2i \operatorname{Im} V \right) dx = 0 . \tag{4}$$

where $\psi ' \equiv \frac{d\psi}{dx}$, and we have assumed $|x_1| < L$ and $|x_2| < L$. Note that for $\psi_1 = \psi_2 \equiv \psi$, Eq. (4) leads back to the following well-known 1D “optical theorem” [2]:

$$j(L) - j(-L) = \frac{\hbar k^2}{mE} \int_{-L}^{L} |\psi|^2 \operatorname{Im} V dx , \tag{5}$$

where $j(x)$ is the probability current density. Using the results in (2) and (3) into (4), it is straightforward to arrive at the following result relating the various reflection and transmission amplitudes:

$$\psi_{1t} \psi_{2r}^* + \psi_{1r} \psi_{2t}^* - \frac{k}{E} \int_{-L}^{L} \psi_1 \psi_2^* \operatorname{Im} V dx = 0 . \tag{6}$$

Now if we apply (1) to both ψ_1 and ψ_2, and using the results in (2) and (3), we can derive a much simpler relation between the various incident and transmission amplitudes as follows:

$$\psi_{1t}\psi_{2i} - \psi_{1i}\psi_{2t} = 0 . \quad (7)$$

By setting both incident amplitudes to be unity (i.e. $\psi_{1i} = \psi_{2i} = 1$), (7) leads back to the guaranteed reciprocal symmetry for transmission which is of general validity:

$$\psi_{1t} = \psi_{2t} \ , \quad (8)$$

and the generalized relation between the reflection amplitudes in (6) can then be rewritten in a slightly different form as follows:

$$\left(\frac{\psi_{2\mathrm{r}}}{\psi_{2\mathrm{t}}}\right)^{*} + \left(\frac{\psi_{1\mathrm{r}}}{\psi_{1\mathrm{t}}}\right) - \frac{k}{E\psi_{1\mathrm{t}}\psi_{2t}^{*}} \int_{-L}^{L} \psi_1 \psi_2^{*} \,\mathrm{Im}\, V dx = 0 . \quad (9)$$

The results in (8) and (9) are the general constraints we seek to derive and are in complete analogy to those obtained in optics by Agarwal and coworkers [8], with Eq. (9) showing that the reflection coefficients (i.e. $\left|\psi_{nr}\right|^2$, n=1,2) are in general different for the left and right incidence in the presence of absorption, i.e. $\mathrm{Im}\,V \neq 0$, a result also well-known in optics (with the dielectric function playing the role of the potential).

However, in the case of a real asymmetric potential, Eq. (9) reduces to:

$$\left(\frac{\psi_{1\mathrm{r}}}{\psi_{1\mathrm{t}}}\right) = -\left(\frac{\psi_{2\mathrm{r}}}{\psi_{2\mathrm{t}}}\right)^{*} , \quad (10)$$

which, together with (8), leads to the well-known result that both the transmission and reflection coefficients are identical for the left and right incidence in the case of a real asymmetric potential [5]. Thus it appears that the asymmetric nature of any real 1D potential cannot be revealed via simple left-versus-right incidence experiment as "protected" by reciprocal symmetry.

Note that all the amplitudes in Eqs. (8) – (10) are in general complex. By writing these in the form of a real amplitude and a phase factor: $\psi = \left|\psi\right| e^{i\phi}$, Eq. (8) shows that both the real amplitudes and phases are identical for the transmitted waves of either the left or the right incidence case. However, Eq. (9) implies that the corresponding relations will in general be rather complicated for the reflected waves. Nevertheless, in the case of *real* potentials, Eqs. (8) and (10) lead in a straightforward way to the following results:

$$|\psi_{1r}| = |\psi_{2r}|, \tag{11}$$

and

$$2\phi_t = \phi_{1r} + \phi_{2r} - \pi \ . \tag{12}$$

While the result in (11) reconfirms the identical reflection coefficients in the two cases of incidence from different sides, that in (12) shows that the phases of the two reflected waves will in general be different --- a result completely analogous to that obtained in Ref. [9] for propagation of optical waves [10]. This result then enables one to identify any asymmetry for a real potential by monitoring any possible deviation from $\pi/2$ in the phase difference between the reflected and the transmitted wave.

Illustrations

In this section, we provide some illustrations of the above general results via direct calculations of the 1D scattering from an asymmetric potential. For simplicity, we shall re-label the amplitudes ψ_r by R and ψ_t by T, and shall divide into two cases:

(I) Case of real potential

Consider the left-incidence case on a real arbitrary potential confined within $0 \le x \le a$ (i.e. $x_1 = 0, x_2 = a$ in Fig. 1(a)), where the wave in the region of the potential is represented by some well-behaved real functions $u(x)$ and $w(x)$, respectively, i.e. the wavefunction in the potential zone is of the form: $\psi_V = Au + Bw$, and the solutions outside the potential are all plane waves. Thus, matching the continuity of the wavefunctions and their derivatives at each of the two boundaries, we finally obtain the following complex amplitudes for the reflection and transmission waves [11]:

$$R_1 = \frac{\left(p_{0a} - p_{a0}\right) - i\left(q - r\right)}{\left(p_{0a} + p_{a0}\right) - i\left(q + r\right)}, \tag{13}$$

$$T_1 = \frac{2}{\left(p_{0a} + p_{a0}\right) - i\left(q + r\right)}, \tag{14}$$

where p_{0a}, p_{a0}, q, and r are all real quantities defined as follows:

$$\left.\begin{aligned} p_{0a} &\equiv u(0)w'(a) - w(0)u'(a) \\ p_{a0} &\equiv u(a)w'(0) - w(a)u'(0) \\ q &\equiv k\left[u(0)w(a) - w(0)u(a)\right] \\ r &\equiv \frac{1}{k}\left[u'(0)w'(a) - w'(0)u'(a)\right] \end{aligned}\right\}. \tag{15}$$

For the right-incidence case as illustrated in Fig. 1(b), one can show in a similar way that the corresponding complex amplitudes are given as follows [7]:

$$R_2 = \frac{\left(p_{a0} - p_{0a}\right) - i\left(q - r\right)}{\left(p_{0a} + p_{a0}\right) - i\left(q + r\right)}, \tag{16}$$

$$T_2 = \frac{2}{\left(p_{0a} + p_{a0}\right) - i\left(q + r\right)}. \tag{17}$$

Thus (16) and (17) show that $T_1 = T_2$, confirming the result in (8); whereas the results in (14) and (16) lead to

$$\frac{R_1}{R_2^*} = -\frac{\left(p_{0a} + p_{a0}\right) + i(q + r)}{\left(p_{0a} + p_{a0}\right) - i(q + r)} = -\frac{T_1}{T_2^*}, \tag{18}$$

where we have used (14) and (17) in the last step. The result in (18) thus reconfirms the result derived in Eq. (10). Furthermore, by expressing the various complex amplitudes as follows:

$$\left.\begin{aligned} &R_1 = |R_1| e^{i\phi_{1r}} \\ &R_2 = |R_2| e^{i\phi_{2r}} = |R_1| e^{i\phi_{2r}} \\ &T_1 = T_2 = |T| e^{i\phi_t} \end{aligned}\right\}, \tag{19}$$

Eq. (18) leads to the following phase relation :

$$e^{i(\phi_{1r}+\phi_{2r})} = -e^{2i\phi_t} \quad \Rightarrow \; \phi_{1r} + \phi_{2r} = \pi + 2\phi_t \ , \tag{20}$$

which reproduces the result given in Eq. (12).

(II) Case of complex potential

Here we perform numerical analysis for a simple asymmetrical potential. In this case, while the results from Eqs. (13) to (17) are still valid, those in (18) and (20) are no longer correct since p_{0a}, p_{a0}, q, and r are now of complex values for the wavefunctions $u(x)$ and $w(x)$ are in general complex. Under this situation, as the general results in the previous section imply, we shall still have reciprocal symmetry for transmission but not for reflection. Instead, the general result in Eq. (9) will set constraints on the reflection amplitudes from the left and right incidence, respectively. To illustrate the validity of Eq. (9), we shall perform some numerical studies of certain specific complex potentials in this section.

Since reciprocity must hold for any symmetric potential, we shall study the simplest potential for which asymmetry of reflection may arise by referring to the two-step potential barrier as indicated in Fig. 1(b). This simple asymmetric potential is of significant interest and has been investigated in the literature for both application [12] and fundamental studies [13].

For simplicity, we shall measure the energy of the electron in units of $(\hbar^2/2m)$ so that $E = k^2$. Also, let potentials V_1 and V_2 be complex (with positive real and imaginary parts), constant, distinct, and of equal width (a) along the x direction. Then within their respective domains, the solution to (1) is:

$$\left.\begin{array}{l}\psi_{V_1} = A_1 e^{ik_1x} + B_1 e^{-ik_1x} \\ \psi_{V_2} = A_2 e^{ik_2x} + B_2 e^{-ik_2x}\end{array}\right\} \qquad (21)$$

The boundary conditions applied to the left-incidence case lead to the following relations among the wave amplitudes:

$$\left.\begin{array}{c}e^{-ika} + R_1 e^{ika} = A_1 e^{-ik_1a} + B_1 e^{ik_1a} \\ ik(e^{-ika} - R_1 e^{ika}) = ik_1(A_1 e^{-ik_1a} - B_1 e^{ik_1a}) \\ A_1 + B_1 = A_2 + B_2 \\ ik_1(A_1 - B_1) = ik_2(A_2 - B_2) \\ T_1 e^{ika} = A_2 e^{ik_2a} + B_2 e^{-ik_2a} \\ ikT_1 e^{ika} = ik_2(A_2 e^{ik_2a} - B_2 e^{-ik_2a})\end{array}\right\}. \qquad (22)$$

Since we make no assumption about reciprocity for the system, the analogous set of equations for the right-incidence must also be solved independently (with $R_1 \to R_2,\ T_1 \to T_2$).

Applying Eq. (9) to this case, we have:

$$\left(\frac{R_2}{T_2}\right)^* + \left(\frac{R_1}{T_1}\right) = (kT_1T_2^*)^{-1}\int_V \psi_1\psi_2^* \operatorname{Im}V dx\,. \qquad (23)$$

Once all the coefficients in (22) have been determined, we may plot the left- and right-hand sides of the above equation as function of the incident energy ($E = k^2$). The results in Figs. 2 and 3 numerically demonstrate the validity of both the real and imaginary parts of (23) for several different potentials. Figs. 2 and 3 are generated by fixing the real parts of each potential step (Re $V_1 = 1$,Re $V_2 = 2$) and plotting the left- and right-hand sides of (23) for several values of the potentials' imaginary parts. In addition, the validity of the phase relation in Eq. (12) is also demonstrated in Fig.4 for real potentials by setting the imaginary parts to zero.

We would like to further comment on the degree of deviation from reciprocity symmetry from the results in Figs. 2 and 3. First we note that the line $y = 0$ in both these figures represent the case of reciprocal symmetry: any deviation from this implies the breakdown of such symmetry. It is clear that within certain limits of the magnitude of the potential's imaginary part, one indeed can see that greater values in this magnitude leads to greater deviations from reciprocity symmetry. However, a monotonic trend does not exist since the quantities plotted in the y-coordinates change sign. Nevertheless, one thing seems quite clear which is that for sufficiently low energies, the absolute value of the deviation from reciprocity symmetry does increase with the magnitude of the imaginary part of the potential, while for very high energy such deviation becomes insignificant.

Discussion and Conclusion

We have in this work studied the reciprocity symmetry of the 1D scattering problem in quantum mechanics for an arbitrary potential (complex and asymmetric). By establishing some generalized relations for the amplitudes and phases between the left-incident and right-incident electron waves, we have shown that even in the most general case of a complex asymmetric potential, the reflected waves from the two cases of incidence are intimately related. Furthermore, in the case of an arbitrary real potential, one can still distinguish the two reflected waves via monitoring the phases in each of them. This provides a possibility of probing an asymmetric non-absorbing potential via interference experiments from beams incident on different sides of the potential.

One also concludes from this study that the transmission symmetry is very strong: it remains valid (both for the amplitude and phase of the two beams) even in the most general case with an asymmetric complex potential [5, 6]. Whereas this strong reciprocal symmetry is also well-known in optics, recent developments in plasmonics and metamaterials have revealed the possibility of breakdown of this symmetry with the propagation of light through these materials [14]. It thus poses an interesting and challenging task for future study to explore similar breakdown of transmission reciprocal symmetry in the propagation of matter waves in quantum mechanics.

Acknowledgments

The authors would like to express their appreciation to Dr. Huai-Yi Xie of the Academia Sinica for his initial efforts in the study of this problem.

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Note that there is a sign error in Eq. (9a) of this paper: the overall sign should be positive rather than negative.

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Figure Captions

1. (a) Geometry of an arbitrary potential.

   (b) A two-step complex potential with positive real and imaginary parts.

2. Demonstration of the validity of the real part of Eq. (23): the curves are results from the LHS of (23) while the dots are obtained from the RHS of (23).

3. Demonstration of the validity of the imaginary part of Eq. (23): the curves are results from the LHS of (23) while the dots are obtained from the RHS of (23).

4. Demonstration of the validity of the phase relation in (12) for real potentials.

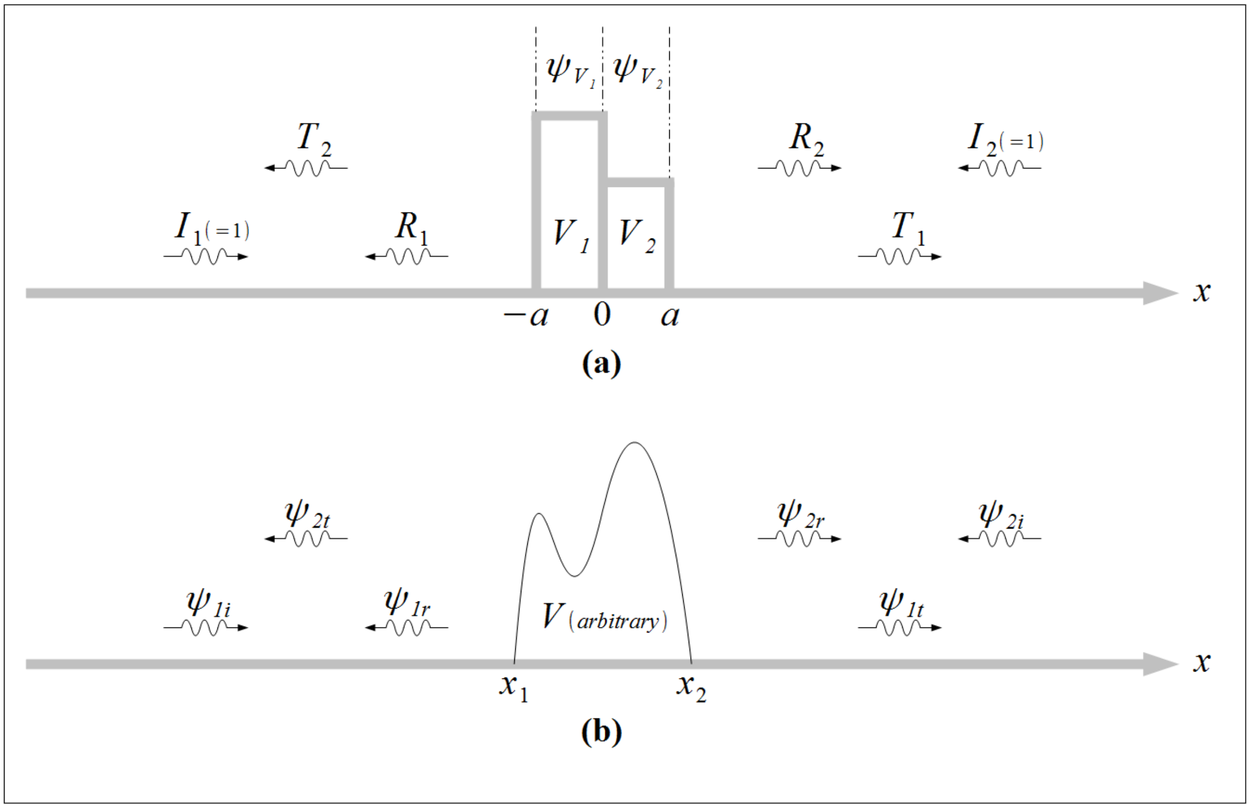
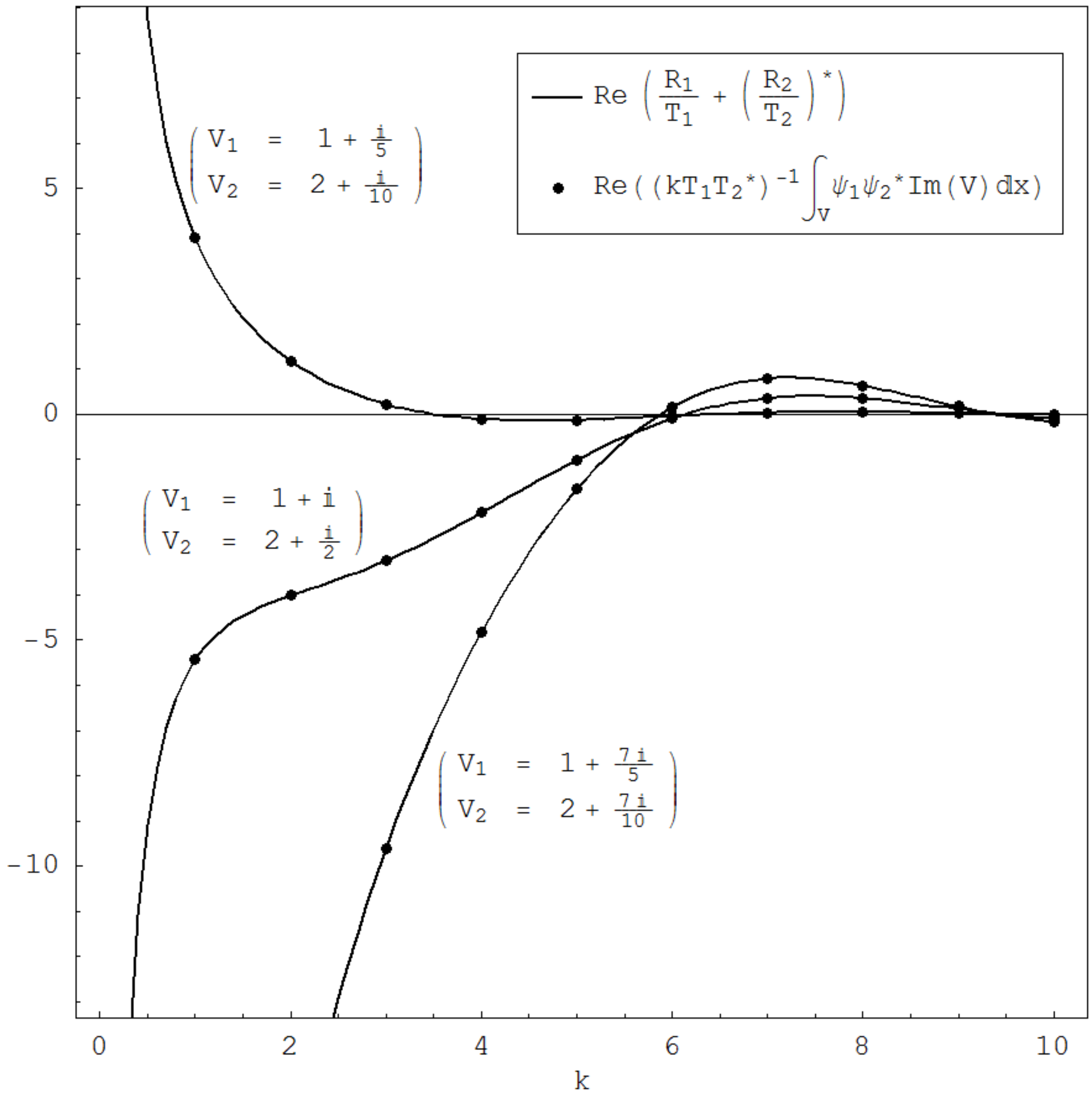

ψ_{V_1}
ψ_{V_2}
T_2
R_2
$I_{2(=1)}$
$I_{1(=1)}$
R_1
V_1
V_2
T_1
x
$-a$
0
a
(a)
ψ_{2t}
ψ_{2r}
ψ_{2i}
ψ_{1i}
ψ_{1r}
$V_{(arbitrary)}$
ψ_{1t}
x
x_1
x_2
(b)

Figure 1



Re $\left(\frac{R_1}{T_1} + \left(\frac{R_2}{T_2}\right)^*\right)$
Re $\left((kT_1T_2^*)^{-1}\int_V \psi_1\psi_2^* \mathrm{Im}(V)\,dx\right)$
$V_1 = 1 + \frac{i}{5}$, $V_2 = 2 + \frac{i}{10}$
$V_1 = 1 + i$, $V_2 = 2 + \frac{i}{2}$
$V_1 = 1 + \frac{7i}{5}$, $V_2 = 2 + \frac{7i}{10}$
5
0
-5
-10
0
2
4
6
8
10
k

Figure 2

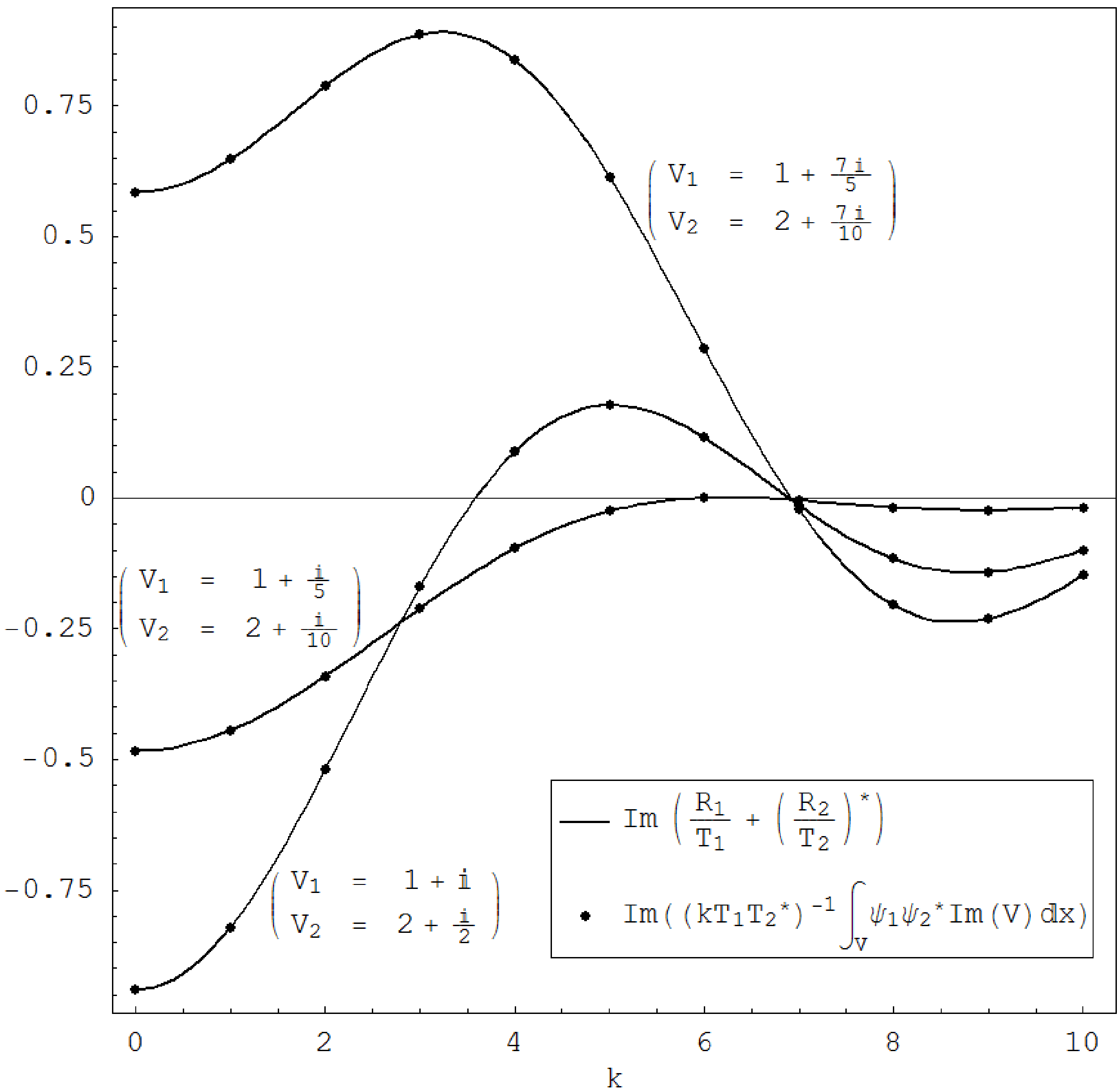

0.75
0.5
0.25
0
-0.25
-0.5
-0.75
0
2
4
6
8
10
k
$V_1 = 1 + \frac{7i}{5}$, $V_2 = 2 + \frac{7i}{10}$
$V_1 = 1 + \frac{i}{5}$, $V_2 = 2 + \frac{i}{10}$
$V_1 = 1 + i$, $V_2 = 2 + \frac{i}{2}$
$\mathrm{Im}\left(\frac{R_1}{T_1} + \left(\frac{R_2}{T_2}\right)^*\right)$
$\mathrm{Im}\left((kT_1T_2^*)^{-1}\int_V \psi_1\psi_2^*\,\mathrm{Im}(V)\,dx\right)$

Figure 3

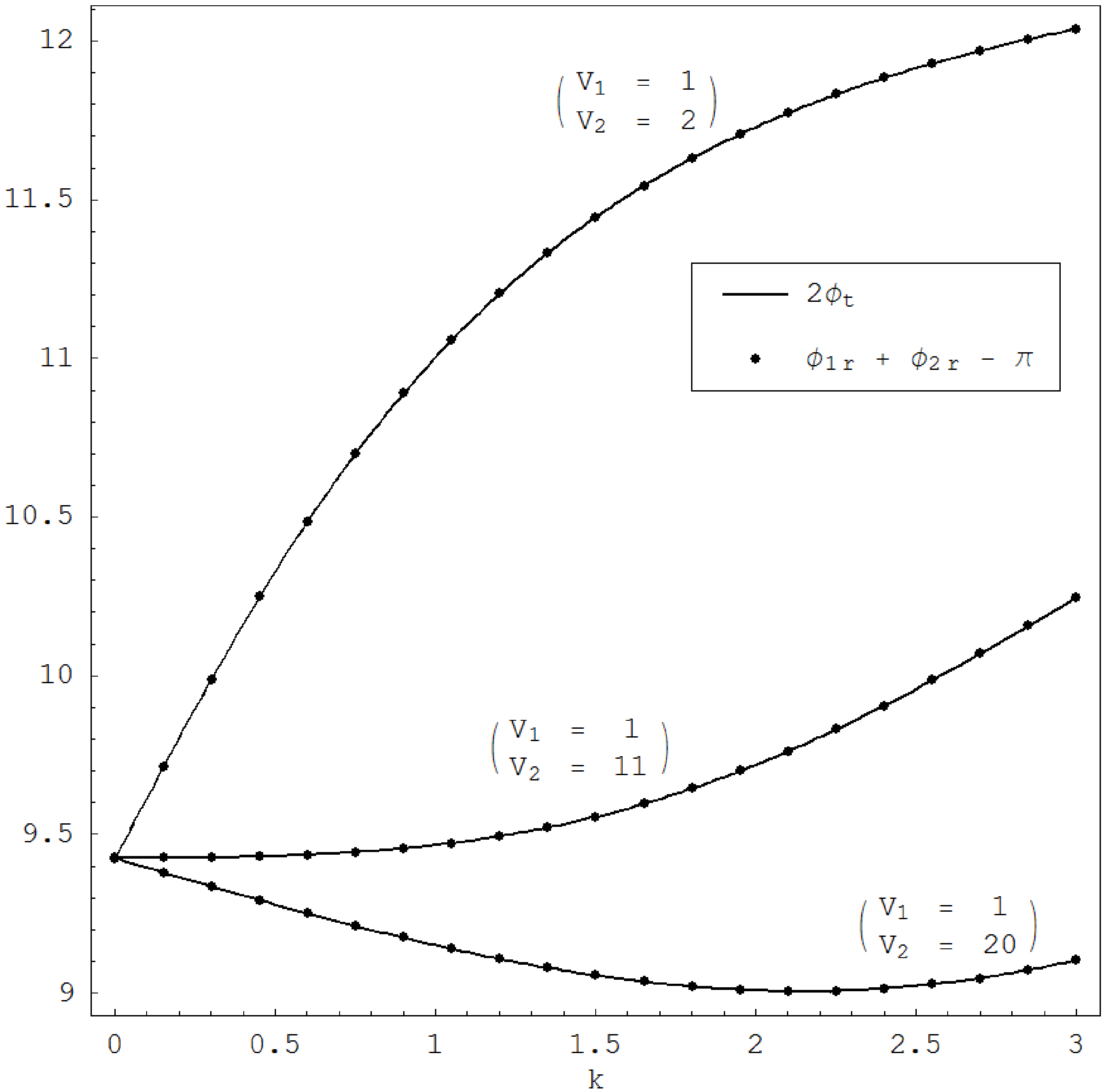

12
11.5
11
10.5
10
9.5
9
0
0.5
1
1.5
2
2.5
3
k
$\begin{pmatrix} V_1 = 1 \\ V_2 = 2 \end{pmatrix}$
$\begin{pmatrix} V_1 = 1 \\ V_2 = 11 \end{pmatrix}$
$\begin{pmatrix} V_1 = 1 \\ V_2 = 20 \end{pmatrix}$
$2\phi_t$
$\phi_{1r} + \phi_{2r} - \pi$

Figure 4