Ramsauer effect in one-dimensional quantum walk with multiple defects

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Experimental observations of quantum walks in one dimension have provided many exciting applications in quantum computing, while recent theoretical investigation of single phase defect in these systems point towards interesting phenomena associated with bound states. Here we obtain analytical solutions of quantum walk with a general quantum coin in one dimension with multiple defects, with new prediction on the condition for zero reflectance for scattering state, and the existence of an analogy to the Ramsauer effect for multiple defects. We also show the transition from the zero reflectance state to the bound state can provide a method for preparing the quantum walk in a bound state. Applications to systems similar to thin film optics are suggested.

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After Feynman's proposal of quantum cellular automaton [1, 2], researchers have introduced a model of discrete time quantum walk [3, 5] which has since become a subject of intense research interest. Theoretically it is a model for universal quantum computation [6, 7] and quantum algorithm [8–11], with relevance in many subjects, such as the topological phases [12], quantum phase transition and localization in optical lattices [13, 14], energy transfer in photosynthetic systems [15, 16], and breakdown of electric field driven systems [17]. Experimental realizations of the discrete time quantum walk are observed in optical resonator [18], nuclear magnetic resonance [19], trapped ions [20, 21] and neutral atoms [22], photons in different structures such as beam splitter array, fiber loop and waveguide [23–31].

In this paper we find an analog of the Ramsauer effect in one-dimensional quantum walk with multiple defects. The Ramsauer effect in quantum mechanics refers to the phenomenon of the probability of electrons tunneling through potential barrier oscillates with respect to energies, and the reflection vanishes at several different energies due to the interference between the incoming wave and the reflecting waves. For one-dimensional quantum walk with defects, we solve for the scattering states as well as bound states and find similar oscillatory behavior in the reflectance.

The simplest soluble model of discrete-time quantum walk [3, 4, 22, 35] is described by iteration of a unitary transformation acting on a two-state particle. The particle is represented by a wave function $|\psi\rangle = \sum_n (a_n |L\rangle + b_n |R\rangle) |n\rangle$ where $|n\rangle$ is the state that quantum walk localized at position $n$ whereas left $|L\rangle$ and right $|R\rangle$ states represent the two internal degree of freedom. Here, $a_n$ and $b_n$ are the left and right components of the wave function at position $n$. The unitary transformation $U = S \cdot C$ consists of a quantum coin operation $C$ that acts on the internal state, followed by a shift operator $S$ to evolve the particle coherently in position space. The shift operator $S$ is $S = |L\rangle\langle L| \sum_n |n\rangle\langle n + 1| + |R\rangle\langle R| \sum_n |n\rangle\langle n - 1|$ which moves the left and right states to the left and right direction by 1 unit respectively. A common example of the coin operator $C$ is Hadamard coin given by,

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{1}$$

where the matrix is written in the basis of $\{|L\rangle, |R\rangle\}$. A general coin operator is a rotation matrix parametrized by a coin parameter $\theta$ as,

$$C = \cos \theta \sigma_x + \sin \theta \sigma_z = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \tag{2}$$

When $\theta = \pi/4$, the general quantum walk reduces to the Hadamard Walk. The simplest solution for one-dimensional quantum walk is plane waves,

$$\psi(n, t) = e^{-iE\epsilon t + iKn} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3}$$

where $E$ and $k$ are the quasi-energy and quasi-momentum with period of $2\pi$ satisfying,

$$\sin E = -\cos \theta \sin k \tag{4}$$

and $a_k$ and $b_k$ are the left and right components of the wave function given by,

$$\begin{pmatrix} a_k \\ b_k \end{pmatrix} = \frac{1}{\sqrt{2 - 2 \cos \theta \cos(E - k)}} \begin{pmatrix} e^{ik} \sin \theta \\ e^{-iE - \cos \theta e^{ik}} \end{pmatrix} \tag{5}$$

For each $E$, there are two possible quasi-momentum $k = -\arcsin(\sin E / \cos \theta)$ and $k = \pi + \arcsin(\sin E / \cos \theta)$ representing waves going to the direction of increasing $n$ or decreasing $n$. The dispersion relation in Eq. 4 is unusual in the sense that the quasi-energies are anti-symmetric with respect to quasi-momentum. This antisymmetry is due to the fact that the coin can never recover the identity matrix by varying $\theta$ parameter, instead, it is reduced to $\sigma_z$ matrix when $\theta = 0$. When $\theta = 0$, the left and right component decoupled. The left component moves to the left without any changing after one unitary transformation which is equivalent to a wave with quasi-momentum $k = 0$ and quasi-energy
$E = 0$ while the right component moves to the right and consistently changes its sign each step which is equivalent to a wave with quasi-momentum $k = \pi$ and quasi-energy $E = 0$. Thus, the wave with $k = 0$ has a negative group velocity and the wave with $k = \pi$ has a positive group velocity when the quasi-energy $E = 0$. For $\theta \in (-\pi/2, \pi/2)$, $\cos \theta$ is positive, thus the group velocity $v_g = dE/dk = -\cos \theta \cos k / \cos E$ is positive for $k \in (\pi/2, 3\pi/2)$ and is negative for $k \in (-\pi/2, \pi/2)$ if we restrict all the discussion to $E \in (-\pi/2, \pi/2)$. On the other hand, for $E \in (\pi/2, 3\pi/2)$, the group velocity changes its direction. In the later discussion, we only study the branch of $E \in (-\pi/2, \pi/2)$.

An extension of this one-dimensional quantum walk model to include a single defect that modifies the phase $\phi$ of the state at the origin $|0\rangle$ was recently investigated by Wojtek et al.\[39\]. Many papers have since been written on this subject.\[40, 41\]. Each time the walker passes through the phase defect $\omega = e^{i\phi}|\phi \in (0, 2\pi)|$ at the origin, it will gain an extra phase $e^{i\phi}$. The unitary transformation with phase defect is $U_\phi = S \cdot e^{i\phi} e^{\omega C}$ and the evolution of this state is governed by $|\Psi(t)\rangle = U_\phi t |\Psi(0)\rangle$.

We first study the scattering state when the incoming wave comes from the negative side, i.e. $k \in (\pi/2, 3\pi/2)$. The defect is treated as a boundary between scattering waves, which is similar to the situation in thin film optics.\[42\]. After hitting on the phase defect, part of the wave transmits through the defect with transmitting amplitude $t$ and the other is reflected with reflecting amplitude $r$ calculated in Appendix A.

$$r = \text{sign}(k - \pi) \frac{(1 - e^{i\phi}) \sqrt{\sin(k - E) \sin(k + E)} (e^{i\phi} - e^{-2iE})}{e^{i\phi} (e^{i\phi} - 1) \sin(E - k) + i(e^{-2iE} - \cos 2k) \cos \theta} + \sin(E + k)(e^{i\phi} - e^{-2iE})$$

$$t = \frac{-\sin(2k) \cos^2 \theta e^{i(\phi - k - E)}}{e^{i\phi} (e^{i\phi} - 1) \sin(E - k) + i(e^{-2iE} - \cos 2k) \cos \theta} + \sin(E + k)(e^{i\phi} - e^{-2iE})$$

where $E$ is a given by Eq. [4] and the sign function is $+1$ for positive variable and $-1$ for negative variable. This sign function is responsible for selecting one of the two branches of the square root function. The unitary transformation $U_\phi$ is invariant under the transformation $\theta \rightarrow \pi - \theta$, the exchange of basis $|L\rangle \leftrightarrow |R\rangle$ and space reversal transformation. The three transformations brings the first equation of the following evolution equations to the second and vice versa,

$$a_{n-1}(t + 1) = \cos \theta a_n(t) + \sin \theta b_n(t)$$
$$b_{n+1}(t + 1) = \sin \theta a_n(t) - \cos \theta b_n(t)$$

Thus the reflecting amplitude, transmitting amplitude and the wave function for the left going wave can be obtained from the right going wave by change $\theta$ to $\pi - \theta$.

Note that $|r|^2 + |t|^2 = 1$. In Fig. [1], we illustrate the contour plot of the reflectance $|r|^2$ of a Hadamard walk, i.e. $\theta = \pi/4$, on the plane of the phase defect $\phi$ and quasi-momentum $k$. When $\phi = 0$, the quantum walk reduces to the situation with no defect and the reflecting amplitude $r$ vanishes. Interestingly, when $\phi = -2E$ corresponding to the 0 level curve in Fig. [1], the reflecting amplitude also vanishes while the transmitting amplitude is $t = e^{-2ik}$. In this situation, quantum walk will transmit with zero reflectance and gain an extra phase $e^{-2ik}$ as if it passes through node 1 coincides with node $-1$. Although the condition for zero reflectance, $\phi = -2E$, is independent of the coin parameter $\theta$, not all phase defects produce zero reflectance phenomena for a given $\theta$. The zero reflectance occurs only when the defect phase is $\phi = -2E = 2\arcsin(\cos \theta \sin k)$ and $k \in (\pi/2, 3\pi/2)$, thus only for $\phi \in (-\pi + 2\theta, \pi - 2\theta)$. For $\phi \in (\pi - 2\theta, 3\pi - 2\theta)$, the reflectance is nearly 1. This range of $\phi$ for zero reflectance agrees with the 0 level curve in Fig. [1] where zero reflectance occurs only in

![FIG. 1. Contour plot of the reflectance of Hadamard walk versus phase shift $\phi$ and quasi-momentum $k$. Darker color represents lower value of reflectance.](image)
critical phase
we show the reflectance versus quasi-momentum at this φ critical phase
non-Hadamard walk, there is a general dependence of the approaches 0 and the reflectance decreases in general. For φ and as − φ critical decreases, the zero reflectance quasi-momentum decreases, the zero reflectance quasi-momentum k becomes a state selector.

FIG. 2. Reflectance of Hadamard walk versus the quasi-momentum k for different φ.

The quasi-momentum dependence of the reflectance |r|^2 for different φ of Hadamard walk is illustrated in Fig. 2. For φ greater than π/2, the critical value for Hadamard walk, zero reflectance state disappears as predicted. Nevertheless, there is still a state with minimum reflectance, which magnitude increases with φ. For − φ critical < φ < φ critical, zero reflectance can be observed and as φ decreases, the zero reflectance quasi-momentum approaches 0 and the reflectance decreases in general. For non-Hadamard walk, there is a general dependence of the critical phase φ critical on the coin parameter θ. In Fig. 3 we show the reflectance versus quasi-momentum at this critical phase φ critical at different θ. When θ = 0.05π, the critical phase φ critical = 0.9π and the overall reflectance is relatively small compared with Hadamard walk; while the critical phase for θ = 0.45π is φ critical = 0.1π and the reflectance is relatively greater. The result shows that the overall reflectance at φ critical increases when θ increases.

It has been shown that bound states may exist for certain φ in Hadamard walk. We now investigate the condition for the existence of bound state using general coin and its transition at critical phase φ. For bound state, the quasi-momentum k is complex so that the wave function decays with distance. Supposing k = −iκ, similar to the calculation for scattering state, by changing the k into −iκ and solving the equations we get four solutions. The details is presented in the Appendix B.

e^{κ±m} = ±i \frac{1}{\sqrt{1 + 2 \sin θ \tan (m) + \tan (θ/2) \tan θ}}\tag{9}

where m = 1, 2. Notice that we have obtained two pairs of bound states with same quasi-energy, κ1± and κ2± while Wojcik et al only obtained two bound states. It is because they study the eigenstate of double-step evolution operator U^2 φ instead of single-step evolution operator U φ. For double-step operator, only the sites differed by distance of 2 are related. Then, e^{κ1+} and e^{κ1−} reduces to same bound state of U^2 φ because the decay rate after distance of 2 for both states are the same, i.e. e^{2κ1+} = e^{2κ1−}. So the four bound states of U φ should reduce to the two bound states of U^2 φ. However, κ1+ bound state and κ1− bound state are different at the odd number sites so they are different states. We therefore conclude that there exist four bound states in quantum walk with single phase defect. Note that bound state exists only when the decay constant e^κ is less than 1, otherwise, the wave function diverges at infinity. From Eq. 9 it can be shown that κ1± bound state exists only when 2π > φ > φ critical = π − 2θ and κ2± bound state exists only when −2π < φ < −φ critical = −π + 2θ.

With both the scattering state and the bound state found, we can consider the transition from one to the other by tuning the defect phase adiabatically. Suppose the quantum walk is prepared in the κ1+ bound state for φ > φ critical = π − 2θ and φ is tuned adiabatically across the critical value φ critical. The bound state will no longer exist but transforms into a right going wave with k = π/2 when φ < φ critical. As φ decreases further, the state becomes the zero reflectance state. This observation is consistent with the fact that zero reflectance

FIG. 3. Reflectance for quantum walk with different θ at critical phase.
defects by first deriving the transition matrix and then apply it to the case with double phase defects. In multiple defects, the wave function is separated into several parts. Between two defects, the wave function is the superposition of left and right going wave with amplitudes $A$, $B$, $C$ and $D$ shown in Fig. 4. When there is a phase defect at position $n = N$, the wave function between the defect and its neighbouring defects is,

$$
\psi(n) = A e^{i k N} a_k + B e^{i (\pi - k) N} b_{\pi - k}, \quad (n < N)
$$

$$
\psi(n) = C e^{i k N} a_k + D e^{i (\pi - k) N} b_{\pi - k}, \quad (n > N)
$$

$$
\psi(N) = \left( C e^{i k N} a_k + D e^{i (\pi - k) N} b_{\pi - k} \right) A e^{i k N} b_k + B e^{i (\pi - k) N} b_{\pi - k}
$$

(10)

By matching the evolution equations at $n = \pm 1$ and rearranging them, the amplitude $A$, $B$, $C$ and $D$ are connected by a matrix $\Lambda(\omega, N)$,

$$
\begin{pmatrix} C \\ D \end{pmatrix} = \Lambda(\omega, N) \begin{pmatrix} A \\ B \end{pmatrix}
$$

(11)

$$
\Lambda(\omega, N) = \begin{pmatrix} e^{-i k N} & 0 \\ 0 & e^{-i (\pi - k) N} \end{pmatrix} \begin{pmatrix} \omega a_k & \omega a_{\pi - k} \\ (\omega - 1) \tan \theta a_k - b_k & (\omega - 1) \tan \theta a_{\pi - k} - b_{\pi - k} \\ (\omega - 1) \tan \theta a_{\pi - k} - b_{\pi - k} & (\omega - 1) \tan \theta b_k - a_k \\ \omega b_k & e^{i (\pi - k) N} \end{pmatrix}^{-1}
$$

(12)

In a system with $n$ defects at $N_i$, $i = 1, \ldots, n$, after transmitting through all the defects, the transmitting amplitude $t$ and reflecting amplitude $r$ are connected through a series multiplication of $\Lambda(\omega_i, N_i)$.

$$
\begin{pmatrix} t \\ 0 \end{pmatrix} = \prod_{i=1}^{n} \Lambda(\omega_i, N_i) \begin{pmatrix} 1 \\ r \end{pmatrix}
$$

(13)

By solving this system of linear equations, the transmitting and reflecting amplitude can be obtained.

We now illustrate this with an example with two defects of same phase $\phi$ at position $n = 0$ and $n = d$ respectively and an oscillatory reflectance that can be shown as an analogue to the Ramsauer effect. Fig. 5 shows the quasi-momentum dependence of the reflectance for Hadamard walk. There are three interesting phenomena. Firstly, the reflectance vanishes at more than one quasi-momentum similar to the Ramsauer effect in quantum mechanics, which says that electrons can perfectly tunnel through the potential barrier for several different energies due to the interference between the incoming wave and the reflecting waves. Secondly, the number of dips of reflectance versus quasi-momentum graphs generally increases with $N$. Thirdly, for $\phi$ from 0 to $\pi$, the larger the $\phi$, the higher the contrast in reflectance.

The similarity between our result for the reflectance of general quantum walk with multiple phase defects and Ramsauer effect suggests that we can actually treat the phase defects in quantum walk as an analogue of delta potentials. The evolution operator of the quantum walk with phase defect differs from evolution operator of the free quantum walk by a factor of $e^{i \phi_0 t}$. It resembles the evolution operator with non-zero potential in quantum mechanics, $U(t) = e^{-i H t} = e^{-i V(t)} U_{\text{free}}(t)$. This points to the interpretation that a phase defect localized at position $n$ is equivalent to a delta potential, $V = -\phi_0 \delta_n$. This interpretation of defect explains the Ramsauer effect in the quantum walk system because it also exists in double delta potential.

One dimensional quantum walk with single phase defect has been solved analytically for the scattering as well as bound states, showing existence of zero reflectance, or total transmittance, when the phase of the phase de-
At different positions, a problem of quantum walk by creating phase defects at rated with periodic lattice of defects. Many phenomena be extended to two and three dimensional lattice, deco-
lation of quantum walk using two-component Dirac quasi-energy will yield zero reflectance. This provides a
ition of the initial state of the quantum walker at several
k of the quasi-momentum
The wave function of a scattering state is,

\[ \psi(n) = e^{i\kappa n} \left( \begin{array}{c} a_k \\ b_k \end{array} \right), \quad (n < 0) \]

\[ = t e^{i\kappa n} \left( \begin{array}{c} a_{\pi-k} \\ b_{\pi-k} \end{array} \right), \quad (n > 0) \]

(A.14)

Thus the wave function at \( n = 0 \) is,

\[ \psi(0) = \left( \begin{array}{c} t a_k \\ b_k + r b_{\pi-k} \end{array} \right) \]  

(A.15)

The transmitting amplitude \( t \) and the reflecting ampli-
tude \( r \) satisfies following system of linear equations,

\[ \omega [\cos \theta t a_k + \sin \theta (b_k + r b_{\pi-k})] = \cos \theta (a_k + r a_{\pi-k}) \]

\[ + \sin \theta (b_{\pi-k}) \]

\[ \omega (\sin \theta t a_k - \cos \theta (b_k + r b_{\pi-k})) = t (\sin \theta a_{\pi-k} + \cos \theta b_{\pi-k}) \]  

(A.16)

The first and second equations come from matching the
left component at \( n = -1 \) and the right component at
\( n = 0 \) respectively. Solving these two equations, we
obtain the reflecting amplitude \( r \) and transmitting am-
plitude \( t \) in Eq. 6 and Eq. 7.

Appendix B. Bound state for one defect

The wave function of the bound states satisfies the
boundary condition at the infinity \( \lim_{n \to \infty} \psi = 0 \). Ac-
ccordingly the quasi-momenta \( \kappa \) becomes a complex vari-
able, thus we introduce a new variable, decay rate \( \kappa = ik \).
Then wave function of the bound state is as follows

\[ \psi(n) = e^{\kappa n} \left( \begin{array}{c} a_k \\ b_k \end{array} \right), \quad (n < 0); \quad \left( \begin{array}{c} t a_{\pi-k} \\ b_k \end{array} \right), \quad (n = 0) \]

\[ = t e^{(i\pi-k)n} \left( \begin{array}{c} a_{i\pi-k} \\ b_{i\pi-k} \end{array} \right), \quad (n > 0) \]

(A.17)

The evolution equations at \( n = \pm 1 \) become the equations of \( \kappa \) and \( t \), a system of non-linear equations,

\[ \omega (\cos \theta t a_{i\pi-k} + \sin \theta b_{i\pi-k}) = \cos \theta a_{\pi-k} + \sin \theta b_k \]

\[ \omega (\sin \theta t a_{i\pi-k} - \cos \theta b_k) = t (\sin \theta a_{\pi-k} + \cos \theta b_{\pi-k}) \]  

(A.18)

The four solutions in Eq. 9 are obtained from solving
these two equations.

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