Decoherence in a one-dimensional quantum walk

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In this article we study decoherence in the discrete-time quantum walk on the line. We generalize the method of decoherent coin quantum walk, introduced by Brun *et al.* [Phys. Rev. A **67**, 32304 (2003)]. Our analytical expressions are applicable for all kinds of decoherence. As an example of the coin-position decoherence, we study the broken line quantum walk and compare our results with the numerical one. We also show that our analytical results reduce to the Brun formalism when only the coin is subjected to decoherence.

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I. INTRODUCTION

The quantum walk (QW) is the quantum analog of the classical random walk (CRW). Notable differences between the QW and the CRW are the quadratic dependency of variance on the number of steps and the complex oscillatory probability distribution in the QW instead of the linear variance dependency and the binomial probability distribution in the CRW. These differences between the QW and the CRW have been used to present several quantum algorithms in order to solve some specific problems [1–6] with performances better than the best known classical versions. Recently Childs has shown that the universal computation can be performed by QW [7] and it is, therefore, another witness of QW importance. Two types of QW have been introduced as the quantum mechanical extension of CRW: *discrete* [8] and *continuous time* [9]. Both have the same result in our problems but finding the relation between them was an open problem for several years. Recently this relation has been found [10,11]. Another classification of QW is based on the network over which the walk takes place. The QW on a line is the simplest possible configuration and has been well studied [8,12–16], but other topologies such as cycles [17,18], two-dimensional lattices [19–23], or n-dimensional hypercubes [24,25] have also been investigated.

Quantum entanglement is another important property of quantum mechanics which has recently attracted much attention in view of its connection with the QW. The effect of entanglement of the coin subspace on the QW [14,21,26], entanglement between the coin and position subspaces [20,27,28], and the QW as the entanglement generators [29,30] are examples of these studies. In addition to all these theoretical studies, experimental implementation and realization of the QW is another interesting subject for researchers [31–36].

In the experimental implementation, the environment effects will be so important, because in practice, the preparation of pure quantum states without interaction with the environment is impossible, and the environment can disturb the quantum states and fade the quantum properties. Therefore it is very important to formulate and quantify the influence of decoherence on the QW and several valuable researches have been done about the decoherent QW [22,33,37–43]. Due to the complexity of the analytical calculations, in most of the previous studies the numerical calculations have been used in investigation of the effects of decoherence on the QW. Although analytical expressions have been driven for some particular cases such as the QW with a coin subject to decoherence [39] or the weak noises case [44], the general analytical formulas with the wide range of use are not found yet. The aim of this article is to generalize the approach of Brun *et al.* [39] and show that such a generalization is applicable for all kinds of decoherence in the one-dimensional discrete-time QW.

This work is organized as follows. Section II gives a brief review on the one-dimensional QW and decoherence. Section III is devoted to drive analytical expressions for the first and second moments in the presence of general decoherence. Our results have then been used in Sec. IV to analyze the *coin-position decoherence* for which separation between the coin noise and the position noise is impossible and, as an example, an analytical calculation on the broken line noise has been presented. An analysis of the *coin decoherence* for which only the coin is subjected to decoherence is also presented in this section and it is shown that our results reduce to the Brun *et al.* formula for the coin decoherence. We summarize our results and present our conclusions in Sec. V.

II. BACKGROUND

From the various methods of studying the effects of decoherence on the quantum systems, the Kraus representation is one of the widely accepted methods [45]. Let us define H_W as the Hilbert space of our system (Walker) and H_E as the Hilbert space of environment spanned by $\{|e_n\rangle\}_{n=0}^{m}$, where m is the dimension of the environment's Hilbert space. In practice, it is not possible to completely isolate the system from the environment, therefore in order to find the time evolution of the system we should consider the time evolution of the whole system (system+environment) and obtain the state of the system by tracing out over the environment's degrees of freedom, i.e.,

$$\rho_{\rm sys} = {\rm Tr}_{\rm Env}(U\rho U^{\dagger}). \qquad (1)$$

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Here U acts both on the system and environment Hilbert spaces. Without loss of generality we assume that the state of the whole system is $\rho = \rho_0 \otimes |env_0\rangle\langle env_0|$. So we can write Eq. (1) as

$$\rho_{\rm sys} = \sum_{n=0}^{m} \langle e_n|U|env_0\rangle \rho_0 \langle env_0|U^\dagger|e_n\rangle = \sum_{n=0}^{m} E_n \rho_0 E_n^\dagger, \tag{2}$$

where $E_n = \langle e_n|U|env_0\rangle$, $n = 0, 1, \ldots, m$, are the so-called Kraus operators. These operators preserve the trace condition, i.e., $\sum_{n=0}^{m} E_n^\dagger E_n = I$.

A. Decoherent one-dimensional QW

QW is the quantum version of the CRW where instead of the coin flipping, we use the coin operator to make superposition on the coin space, and instead of the walking in CRW we use the translation operator to move quantum particle according to the coin's degrees of freedom.

In one-dimensional QW we have two degrees of freedom in the coin space H_c, spanned by $\{|L\rangle, |R\rangle\}$, and infinite degrees of freedom in the position space H_p, spanned by $\{|i\rangle \; i = -\infty, \ldots, \infty\}$. The whole Hilbert space of the walker is defined as the tensor product of the coin space H_c and the position space H_p, i.e., $H = H_p \otimes H_c$. In one step of the QW we first make superposition on the coin space with the coin operator U_c and after that we move the particle according to the coin state with the translation operator S as follows

$$U_w = S(I \otimes U_c), \tag{3}$$

where

$$S = \sum_x |x+1\rangle\langle x| \otimes |R\rangle\langle R| + |x-1\rangle\langle x| \otimes |L\rangle\langle L|. \tag{4}$$

Therefore the quantum walking is defined by

$$|\Psi(t+1)\rangle = U_w|\Psi(t)\rangle \rightarrow |\Psi(t)\rangle = {U_w}^t|\Psi(0)\rangle. \tag{5}$$

In ideal case that one can isolate the system from the environment perfectly, the time evolution of the system takes place coherently and the state of the walker remains pure after t steps of the walking. But in the real world where the interaction between the system and the environment is unavoidable, the purity of the system is decreased and the state of the walker becomes mixed. In this case we should consider the evolution of the whole system, i.e, system+environment, defined on the Hilbert space

$$H = H_E \otimes H_p \otimes H_c. \tag{6}$$

By definition of the Kraus operators, one step of the walking can be written as follows

$$\rho(t+1) = \sum_{n=0}^{m} E_n \rho(t) E_n^\dagger. \tag{7}$$

For t steps, we can write

$$\rho(t) = \sum_{n_t=0}^{m} \cdots \sum_{n_2=0}^{m} \sum_{n_1=0}^{m} E_{n_t} \cdots E_{n_2} E_{n_1} \rho(0) E_{n_1}^\dagger E_{n_2}^\dagger \cdots E_{n_t}^\dagger. \tag{8}$$

It is worth noting that the Eq. (8) is general and the Kraus operators E_n include the whole information of all types of evolution. It follows, therefore, that the coin operator, the translation operator and the environment effects all are embedded in E_n and we did not assume any restriction yet.

The Kraus operators satisfy an important constraint known as *completeness relation* [45] which arise from the fact that the trace of $\rho(t+1)$ must be equal to one, i.e.

$$\begin{aligned} 1 = \mathrm{Tr}(\rho(t+1)) &= \mathrm{Tr}\left[\sum_n E_n \rho(t) {E_n}^\dagger\right] \\ &= \mathrm{Tr}\left[\sum_n {E_n}^\dagger E_n \rho(t)\right]. \end{aligned} \tag{9}$$

Since this is true for all ρ then

$$\sum_n {E_n}^\dagger E_n = I. \tag{10}$$

To make any progress we should therefore find the Kruse operators for our system defined in Eq. (2), and use Eq. (8) in order to obtain the final state $\rho(t)$. Evidently, the E_n are operators that act on the system (coin+position) Hilbert space, and therefore we can write the general form of E_n as follows

$$\begin{aligned} E_n &= \sum_{x,x'} \sum_{i,j} a^{(n)}_{x,x',i,j} |x'\rangle\langle x| \otimes |i\rangle\langle j| \\ &= \sum_x \sum_l \sum_{i,j} a^{(n)}_{x,l,i,j} |x+l\rangle\langle x| \otimes |i\rangle\langle j|, \end{aligned} \tag{11}$$

where $x, l = -\infty, \ldots, \infty$ and $i, j = \{L, R\}$.

In the following section we show that a reasonable suggestion on the coefficient $a^{(n)}$ of Eq. (11) enables us to derive useful analytical expression for the first and second moments of position.

B. Environment effects (decoherence)

In this section we briefly discuss the interpretation of noisy evolution and the Kraus representation. Assume that the p_i is the probability that the ith unknown reason affects the state of the system. In other words, the evolution operators A_i act on the system with the corresponding probabilities p_i.

Now we are interested in the walker, though the unitary evolution takes place in the Hilbert space of the system+environment, given in Eq. (6). Furthermore the environment could be the rest of the universe, so determining the exact reasons needs the investigation of the whole universe which is impossible.

Fortunately, in practice, understanding of the exact form of the environment is not required. Let us assume that we have r different operators A_i, $i = 1, \ldots, r$, where each of them acts on the system with the probability p_i. If the environment be in the state $|e_i\rangle$ then the operator A_i acts on the system. Therefore, we can imagine the r-dimensional Hilbert space for the environment, spanned by $\{|e_i\rangle\}_{i=1}^r$, and the following initial state for the environment

$$|env_0\rangle = \sqrt{p_1}|e_1\rangle + \sqrt{p_2}|e_2\rangle + \cdots + \sqrt{p_r}|e_r\rangle. \tag{12}$$

It is clear that the probability of finding the environment in the state $|e_i\rangle$ is p_i. Therefore we can write the unitary transformation of the whole system (environment+system) as follows

$$U = |e_1\rangle\langle e_1| \otimes A_1 + |e_2\rangle\langle e_2| \otimes A_2 + \cdots + |e_r\rangle\langle e_r| \otimes A_r. \tag{13}$$

So the Kraus operators will be

$$E_i = \langle e_i|U|env_0\rangle = \sqrt{p_i}A_i. \tag{14}$$

Accordingly, the Eq. (7) gives the density matrix after the first step as

$$\rho' = \sum_{i=1}^{r} E_i\rho E_i^\dagger = \sum_{i=1}^{r} p_i A_i \rho A_i^\dagger. \tag{15}$$

As we see, this is exactly our expectation from the influence of noise because it gives ρ' as a mixture of different evolutions with the corresponding probabilities p_i. With Eqs. (12) and (13) we can represent the effects of noise by the Kraus operators.

III. FORMALISM

The Fourier transformation is a powerful tool for analytical investigation of the one-dimensional QW, where is defined as follows

$$|x\rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikx}|k\rangle. \tag{16}$$

Using this transformation we can write Eq. (11) in k space as

$$\tilde{E}_n = \sum_{x,l}\sum_{i,j} a^{(n)}_{x,l,i,j} \iint \frac{dkdk'}{4\pi^2} e^{-ilk} e^{-ix(k-k')}|k\rangle\langle k'| \otimes |i\rangle\langle j|. \tag{17}$$

In the following we assume that the coefficients $a^{(n)}_{x,l,i,j}$ are not dependent on the coordinate x. This means that the probability of translation in the position space depends only on the length l of the translation, not on the position x where the translation takes place. In view of this constraint on the $a^{(n)}$, we are able to derive an analytical expression for the first and second moments of the position, which is applicable for a large family of decoherence in the one-dimensional QW. In this regime, the Eq. (17) takes the following form

$$\tilde{E}_n = \sum_{l}\sum_{i,j} a^{(n)}_{l,i,j} \iint \frac{dkdk'}{2\pi^2} e^{-ilk}\delta(k-k')|k\rangle\langle k'| \otimes |i\rangle\langle j|, \tag{18}$$

where we have used the orthonormalization relation

$$\sum_x e^{-ix(k-k')} = 2\pi\delta(k-k'). \tag{19}$$

By integration on k' and changing the order of integration and summation we get

$$\tilde{E}_n = \int \frac{dk}{2\pi}|k\rangle\langle k| \otimes C_n(k), \tag{20}$$

where

$$C_n(k) = \sum_l \sum_{i,j} a^{(n)}_{l,i,j} e^{-ilk}|i\rangle\langle j|. \tag{21}$$

Now by writing the general form of ρ_0 in the k space as

$$\rho_0 = \iint \frac{dkdk'}{4\pi^2}|k\rangle\langle k'| \otimes |\psi_0\rangle\langle\psi_0| \tag{22}$$

the first step of walking from Eq. (7) becomes

$$\begin{aligned}\rho' &= \iint \frac{dkdk'}{4\pi^2}|k\rangle\langle k'| \otimes \sum_n C_n(k)|\psi_0\rangle\langle\psi_0|C_n^\dagger(k') \\ &= \iint \frac{dkdk'}{4\pi^2}|k\rangle\langle k'| \otimes \mathcal{L}_{k,k'}|\psi_0\rangle\langle\psi_0|,\end{aligned} \tag{23}$$

where $\mathcal{L}_{k,k'}$ is a superoperator defined by

$$\mathcal{L}_{k,k'}\tilde{O} = \sum_n C_n(k)\tilde{O}C_n^\dagger(k'). \tag{24}$$

Therefore after t steps, the state of the walker and the probability of finding the walker in position x are, respectively,

$$\rho(t) = \iint \frac{dkdk'}{4\pi^2}|k\rangle\langle k'| \otimes \mathcal{L}^t_{k,k'}|\psi_0\rangle\langle\psi_0| \tag{25}$$

and

$$\begin{aligned}p(x,t) &= \iint \frac{dkdk'}{4\pi^2}\langle x|k\rangle\langle k'|x\rangle \mathrm{Tr}\big(\mathcal{L}^t_{kk'}\rho_0\big) \\ &= \iint \frac{dkdk'}{4\pi^2} e^{-ix(k'-k)}\mathrm{Tr}\big(\mathcal{L}^t_{kk'}\rho_0\big).\end{aligned} \tag{26}$$

Note that the completeness relation given in Eq. (10) implies that

$$\sum_n C_n^\dagger(k)C_n(k) = I. \tag{27}$$

It follows from this condition on the coin operator that the superoperators $\mathcal{L}_{k,k}$ are *trace preserving*, i.e.,

$$\begin{aligned}\mathrm{Tr}(\mathcal{L}_{k,k}\tilde{O}) &= \mathrm{Tr}\left(\sum_n C_n(k)\tilde{O}C_n^\dagger(k)\right) \\ &= \mathrm{Tr}\left(\sum_n C_n^\dagger(k)C_n(k)\tilde{O}\right) = \mathrm{Tr}(\tilde{O})\end{aligned} \tag{28}$$

and therefore

$$\mathrm{Tr}\big(\mathcal{L}^m_{k,k}\tilde{O}\big) = \mathrm{Tr}(\tilde{O}), \tag{29}$$

which are true for arbitrary operator $\tilde{O}$.

Evidently if we know the operators $C_n(k)$, the state and the probability distribution of the system can be obtained by direct using of Eqs. (25) and (26). But unfortunately it is these equations which are difficult to handle, and therefore we turn our attention on the *moments* of this distribution. The mth moment of the probability distribution $p(x,t)$ is defined by

$$\langle x^m\rangle = \sum_x x^m p(x,t). \tag{30}$$

Inserting Eq. (26) in Eq. (30) we get

$$\langle x^m\rangle = \frac{1}{4\pi^2}\sum_x x^m \iint dkdk' e^{-ix(k'-k)}\mathrm{Tr}\big(\mathcal{L}^t_{kk'}\rho_0\big). \tag{31}$$

Using the orthonormalization relation (19), we get for the moments $\langle x\rangle$ and $\langle x^2\rangle$

$$\begin{aligned}\langle x\rangle &= \frac{-i}{2\pi}\iint dk dk' \frac{d\delta(k'-k)}{dk}\mathrm{Tr}\big(\mathcal{L}^t_{kk'}\rho_0\big)\\ \langle x^2\rangle &= \frac{1}{2\pi}\iint dk dk' \frac{d^2\delta(k'-k)}{dk'dk}\mathrm{Tr}\big(\mathcal{L}^t_{kk'}\rho_0\big).\end{aligned} \tag{32}$$

In order to carry out these integrations we need the following equations

$$\begin{aligned}\frac{d}{dk}\mathrm{Tr}(\mathcal{L}_{kk'}\tilde{O}) &= \mathrm{Tr}\left(\sum_n \frac{dC_n(k)}{dk}\tilde{O}C^\dagger_n(k')\right)\\ \frac{d}{dk'}\mathrm{Tr}(\mathcal{L}_{kk'}\tilde{O}) &= \mathrm{Tr}\left(\sum_n C_n(k)\tilde{O}\frac{dC^\dagger_n(k')}{dk'}\right)\end{aligned} \tag{33}$$

where according to Eq. (21)

$$\begin{aligned}\frac{dC_n(k)}{dk} &= -i\sum_l\sum_{i,j} l a^{(n)}_{l,i,j} e^{-ilk}|i\rangle\langle j|\\ \frac{dC^\dagger_n(k')}{dk'} &= i\sum_l\sum_{i,j} l\big(a^{(n)}_{l,i,j}\big)^* e^{ilk'}|j\rangle\langle i|.\end{aligned} \tag{34}$$

Since the superoperator $\mathcal{L}_{k,k'}$ acts on the density matrix which is positive and Hermitian, we can write the Eq. (33) as follows

$$\begin{aligned}\frac{d}{dk}\mathrm{Tr}(\mathcal{L}_{kk'}\rho) &= \mathrm{Tr}(\mathcal{G}_{kk'}\rho)\\ \frac{d}{dk'}\mathrm{Tr}(\mathcal{L}_{kk'}\rho) &= \mathrm{Tr}(\mathcal{G}^\dagger{}_{k'k}\rho),\end{aligned} \tag{35}$$

where

$$\mathcal{G}_{k,k'}\tilde{O} = \sum_n \frac{dC_n(k)}{dk}\tilde{O}C^\dagger_n(k'). \tag{36}$$

Finally by carrying out the integrations of Eq. (32) and putting everything together, we arrive at the following relations for the first and second moments

$$\begin{aligned}\langle x\rangle_t &= i\int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{m=1}^{t}\mathrm{Tr}\big\{\mathcal{G}_k\big(\mathcal{L}^{m-1}_k|\psi_0\rangle\langle\psi_0|\big)\big\}\\ \langle x^2\rangle_t &= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{m=1}^{t}\sum_{m'=1}^{m-1}\mathrm{Tr}\big\{\mathcal{G}^\dagger_k\mathcal{L}^{m-m'-1}_k\big(\mathcal{G}_k\mathcal{L}^{m'-1}_k|\psi_0\rangle\langle\psi_0|\big)\\ &\quad+\mathcal{G}_k\mathcal{L}^{m-m'-1}_k\big(\mathcal{G}^\dagger_k\mathcal{L}^{m'-1}_k|\psi_0\rangle\langle\psi_0|\big)\big\}\\ &\quad+\int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{m=1}^{t}\mathrm{Tr}\big\{\mathcal{J}_k\big(\mathcal{L}^{m-1}_k|\psi_0\rangle\langle\psi_0|\big)\big\},\end{aligned} \tag{37}$$

where we have defined

$$\mathcal{J}_k = \frac{d\mathcal{G}^\dagger_{k,k'}}{dk}\bigg|_{k'=k} = \sum_n\frac{dC_n(k)}{dk}\tilde{O}\frac{dC^\dagger_n(k')}{dk'}\bigg|_{k'=k} \tag{38}$$

and have used $\mathcal{L}_k \equiv \mathcal{L}_{k,k}$ and $\mathcal{G}_k \equiv \mathcal{G}_{k,k}$ for the sake of simplicity. It is worth noting that thus obtained moments in Eq. (37) are a generalization of the moments given by Brun *et al.* in Ref. [39], in the sense that they are applicable for all kinds of decoherence.

IV. CALCULATIONS AND RESULTS

In this section our task is to show that the method is applicable for all possible kinds of decoherence. To this aim, in the first subsection we consider the broken line decoherence as an example of the coin-position decoherence for which we cannot separate the coin noise from the position noise. In the second subsection, we restrict ourselves to the case that the coin is subjected to decoherence but the position is free of noise and show that our method reduces to the result of Brun *et al.* given in Ref. [39].

A. Coin-position decohrence

In this subsection we investigate the effects of coin-position decoherence on the QW. As an example of our approach we find the diffusion coefficient of the one-dimensional QW in the presence of broken line noise. This model has been studied by Romanelli *et al.* [42], where the authors have calculated the diffusion coefficient numerically. They have introduced broken line decoherence for the one-dimensional QW in such a way that the connection between neighbors of current position breaks with probability p, i.e., the walker does not walk with probability p. It turns out that with probability $(1-p)^2$ both links are connected and the walker proceeds normally. On the other hand, with probability $p(1-p)$ (res. p^2) one line (res. both lines) is broken and the walker is returned back (res. is stopped) (see Fig. 1).

Let us rename S in Eq. (4) to S_1 as the translation operator for the case that we don't have any broken line. We also define the translation operators S_2, S_3, S_4 for the cases that the left,

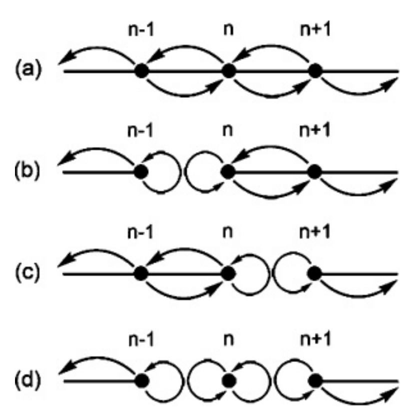

FIG. 1. Possible situations for site n when there are (a) no broken links, (b) the link to the left of the site is broken, (c) the link to the right of the site is broken, and (d) both links are broken. The arrows indicate the direction of the probability flux associated to the L,R components.

right, and both lines are broken, respectively, i.e.

$$\begin{aligned}
S_1 &= \sum_x |x+1\rangle\langle x| \otimes |R\rangle\langle R| + e^{i\theta_1}|x-1\rangle\langle x| \otimes |L\rangle\langle L| \\
S_2 &= \sum_x |x+1\rangle\langle x| \otimes |R\rangle\langle R| + e^{i\theta_2}|x\rangle\langle x| \otimes |R\rangle\langle L| \\
S_3 &= \sum_x |x\rangle\langle x| \otimes |L\rangle\langle R| + e^{i\theta_3}|x-1\rangle\langle x| \otimes |L\rangle\langle L| \\
S_4 &= \sum_x |x\rangle\langle x| \otimes (|R\rangle\langle L| + e^{i\theta_4}|L\rangle\langle R|).
\end{aligned} \tag{39}$$

The situations corresponding to the above translation operators are demonstrated in Fig. 1. Note that we have used the general phase for each translation operator. Later we will see that we need these generic phases in order to have the correct physical phenomena.

As mentioned before, the environment state determines the broken line situation. For instance, if the environment is in the state $|e_1\rangle$, then S_1 acts on the system and so on. Therefore, according to the Eq. (12) we can define the initial state of the environment as follows

$$|env_0\rangle = (1-p)|e_1\rangle + \sqrt{p(1-p)}(|e_2\rangle + |e_3\rangle) + p|e_4\rangle. \tag{40}$$

Also from Eqs. (3) and (13), the general unitary transformation of the system-environment is as follows

$$\begin{aligned}
U &= |e_1\rangle\langle e_1| \otimes S_1(I\otimes H) + |e_2\rangle\langle e_2| \otimes S_2(I\otimes H) \\
&\quad + |e_3\rangle\langle e_3| \otimes S_3(I\otimes H) + |e_4\rangle\langle e_4| \otimes S_4(I\otimes H),
\end{aligned} \tag{41}$$

where we have assumed the Hadamard walk, i.e., $U_c = H$. Therefore according to Eq. (13) $A_i = S_i(I\otimes H)$, and we find from Eq. (14) the Kraus operators as

$$\begin{aligned}
E_1 &= (1-p)\sum_x |x+1\rangle\langle x| \otimes |R\rangle\langle R|H \\
&\quad + e^{i\theta_1}|x-1\rangle\langle x| \otimes |L\rangle\langle L|H
\end{aligned} \tag{42}$$

$$\begin{aligned}
E_2 &= \sqrt{p(1-p)}\sum_x |x+1\rangle\langle x| \otimes |R\rangle\langle R|H \\
&\quad + e^{i\theta_2}|x\rangle\langle x| \otimes |R\rangle\langle L|H
\end{aligned} \tag{43}$$

$$\begin{aligned}
E_3 &= \sqrt{p(1-p)}\sum_x |x\rangle\langle x| \otimes |L\rangle\langle R|H \\
&\quad + e^{i\theta_3}|x-1\rangle\langle x| \otimes |L\rangle\langle L|H
\end{aligned} \tag{44}$$

$$E_4 = p\sum_x |x\rangle\langle x| \otimes (|R\rangle\langle L|H + e^{i\theta_4}|L\rangle\langle R|H). \tag{45}$$

All of these operators are in the form given by Eq. (11). For instance, the coefficients $a^{(1)}$ for E_1 are

$$\begin{aligned}
a^{(1)}_{1,R,R} &= \frac{1-p}{\sqrt{2}} \quad a^{(1)}_{-1,L,L} = -e^{i\theta_1}\frac{1-p}{\sqrt{2}} \\
a^{(1)}_{1,R,L} &= \frac{1-p}{\sqrt{2}} \quad a^{(1)}_{-1,L,R} = e^{i\theta_1}\frac{1-p}{\sqrt{2}},
\end{aligned} \tag{46}$$

where can be used in Eq. (21) and obtain C_1 as

$$C_1 = \frac{1-p}{\sqrt{2}}\begin{pmatrix} e^{-ik} & e^{-ik} \\ e^{i(k+\theta_1)} & -e^{i(k+\theta_1)} \end{pmatrix}. \tag{47}$$

Similarly, we can find the other C_i as follows

$$\begin{aligned}
C_2 &= \sqrt{\frac{1-p}{2}}\begin{pmatrix} e^{-ik}+e^{i\theta_2} & e^{-ik}-e^{i\theta_2} \\ 0 & 0 \end{pmatrix} \\
C_3 &= \sqrt{\frac{1-p}{2}}\begin{pmatrix} 0 & 0 \\ 1+e^{i(k+\theta_3)} & 1-e^{i(k+\theta_3)} \end{pmatrix} \\
C_4 &= \frac{p}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ e^{i\theta_4} & e^{i\theta_4} \end{pmatrix}.
\end{aligned} \tag{48}$$

These C_i must satisfy the completeness relation given by Eq. (27). After some calculations we find that for any θ_1, θ_4 but only when $\theta_2 - \theta_3 = \pi$, Eq. (27) is satisfied. In the following, for simplicity, we choose $\theta_1 = \theta_3 = \theta_4 = 0$ and $\theta_2 = \pi$.

According to Eq. (24), with these C_i in hands, we can find the superoperator $\mathcal{L}_{k,k'}$. But as we know, we have to calculate the mth power of this superoperator which is not an easy task to handle. To get around this complexity, we follow the method of Ref. [39] and use the *affine map* approach. Since the $\mathcal{L}_k$ is linear we can represent it as a matrix acting on the space of two-by-two operators. To do this we note that one can represent any two-by-two matrix by a four-dimensional column vector as

$$\tilde{O} = r_0 I + r_1\sigma_1 + r_2\sigma_2 + r_3\sigma_3 \equiv \begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix}, \tag{49}$$

where

$$r_i = \tfrac{1}{2}\mathrm{Tr}(\sigma_i \tilde{O}). \tag{50}$$

Here we have defined $\sigma_0 = I$, and σ_i $(i = 1, 2, 3)$ are the usual Pauli matrices.

Now, in order to find the superoperators $\mathcal{L}_k$, $\mathcal{G}_k$, $\mathcal{G}_k^\dagger$, and $\mathcal{J}_k$, we represent the action of them on an arbitrary two-by-two matrix $\tilde{O}$ as follows

$$\mathcal{L}_k\tilde{O} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & e & f+p^2 \\ 0 & 0 & -f+p^2 & e \\ 0 & 1-2p & -2g & -2h \end{pmatrix}\begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix} \tag{51}$$

$$\mathcal{G}_k\tilde{O} \equiv \begin{pmatrix} 0 & i(p-1) & ig & ih \\ 0 & 0 & f & -e \\ 0 & 0 & e & f \\ i(p-1) & 0 & -h & g \end{pmatrix}\begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix} \tag{52}$$

$$\mathcal{J}_k\tilde{O} \equiv \begin{pmatrix} 1-p & 0 & 0 & 0 \\ 0 & 0 & -e & -f \\ 0 & 0 & f & -e \\ 0 & 1-p & 0 & 0 \end{pmatrix}\begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix} \tag{53}$$

and

$$\mathcal{G}_k^\dagger\tilde{O} = \mathcal{G}_k^*\tilde{O}, \tag{54}$$

where the last is obtained, simply, from the Hermiticity of the Pauli matrices. Here e, f, g, and h are functions of p and k, defined by

$$\begin{aligned} e(p,k) &= (p-1)^2 \sin(2k) \\ f(p,k) &= (p-1)^2 \cos(2k) \\ g(p,k) &= p(1-p)\sin(k) \\ h(p,k) &= p(1-p)\cos(k). \end{aligned} \tag{55}$$

With this representation we can calculate the moments given by Eq. (37). Since $\mathrm{Tr}(\mathcal{L}_k\tilde{O}) = 2r_0$ and the $\mathcal{L}_k$ is trace preserving, so it does not change r_0. Therefore the only nontrivial result arises from the following three-by-three submatrix

$$M_k = \begin{pmatrix} 0 & e & f+p^2 \\ 0 & -f+p^2 & e \\ 1-2p & -2g & -2h \end{pmatrix}. \tag{56}$$

For finding $\langle x\rangle$ in Eq. (37) we should take trace, accordingly, only the first row of $\mathcal{G}_k$ is important

$$\langle x\rangle_t = \frac{-1}{\pi}\int_{-\pi}^{\pi} dk\big((p-1)\ g\ h\big)\left[\sum_{m=1}^{t} M_k^{m-1}\right]\begin{pmatrix} r_1 \\ r_2 \\ r_3\end{pmatrix}. \tag{57}$$

We can use the geometric progression to simplify the summation in this equation.

$$\langle x\rangle_t \approx \frac{-1}{\pi}\int_{-\pi}^{\pi} dk\big((p-1)\ g\ h\big)[(I-M_k)^{-1}]\begin{pmatrix} r_1 \\ r_2 \\ r_3\end{pmatrix}. \tag{58}$$

Note that we omit the M_k^t in this equation because all eigenvalues of M_k obey $0 < |\lambda| < 1$ and $M_k^t \to 0$ in long time limit. All t dependence has vanished; therefore, in long time limit the first moment is time independent.

The matrix $(I - M_k)$ is exactly invertible and calculation of $\langle x\rangle_t$ is straightforward but our interest is finding the diffusion coefficient with below definition

$$D = \frac{1}{2}\lim_{t\to\infty}\frac{\partial\sigma^2}{\partial t}, \tag{59}$$

where $\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$. Clearly the time independent term does not contribute to D, therefore we focus on finding the second moment in Eq. (37). To begin with, let us first calculate the last term of $\langle x^2\rangle_t$, i.e.,

$$\int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{m=1}^{t}\mathrm{Tr}\big\{\mathcal{J}_k\big(\mathcal{L}_k^{m-1}|\psi_0\rangle\langle\psi_0|\big)\big\}. \tag{60}$$

Since only the first row of $\mathcal{J}_k$ [Eq. (53)] makes nonzero result in the trace, therefore

$$\int_{-\pi}^{\pi}\frac{dk}{\pi}\sum_{m=1}^{t}(\,1-p\ 0\ 0\ 0)\mathcal{L}_k^{m-1}\begin{pmatrix} 1/2 \\ r_1 \\ r_2 \\ r_3\end{pmatrix} = (1-p)t, \tag{61}$$

where we put $r_0 = 1/2$ because of the normalization condition of $|\psi_0\rangle$. Now we turn our attention to the first term of $\langle x^2\rangle_t$ in Eq. (37), i.e.,

$$\begin{aligned} &= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{m=1}^{t}\sum_{m'=1}^{m-1}\mathrm{Tr}\big\{\mathcal{G}_k^\dagger\mathcal{L}_k^{m-m'-1}\big(\mathcal{G}_k\mathcal{L}_k^{m'-1}|\psi_0\rangle\langle\psi_0|\big) + \mathcal{G}_k\mathcal{L}_k^{m-m'-1}\big(\mathcal{G}_k^\dagger\mathcal{L}_k^{m'-1}|\psi_0\rangle\langle\psi_0|\big)\big\} \\ &= -i\int_{-\pi}^{\pi}\frac{dk}{\pi}\sum_{m=1}^{t}\sum_{m'=1}^{m-1}\big(0\ (p-1)\ g\ h\big)\mathcal{L}_k^{m-m'-1}(\mathcal{G}_k-\mathcal{G}_k^\dagger)\mathcal{L}_k^{m'-1}\begin{pmatrix} 1/2 \\ r_1 \\ r_2 \\ r_3\end{pmatrix}, \end{aligned} \tag{62}$$

where in the second line we use the facts that only the first row of $\mathcal{G}_k$ and $\mathcal{G}_k^\dagger$ makes nonzero result in the trace and that the first row of $\mathcal{G}_k$ is pure imaginary.

Since the $\mathcal{L}_k$ is trace preserving and leaves r_0 unchanged, we write

$$\mathcal{L}_k^{m'-1}\begin{pmatrix} 1/2 \\ r_1 \\ r_2 \\ r_3\end{pmatrix} = \begin{pmatrix} 1/2 \\ r_1' \\ r_2' \\ r_3'\end{pmatrix}. \tag{63}$$

Also from Eqs. (52) and (54) we find the exact form of $\mathcal{G}_k - \mathcal{G}_k^\dagger$ as

$$(\mathcal{G}_k - \mathcal{G}_k^\dagger)\tilde{O} = 2i\begin{pmatrix} 0 & (p-1) & g & h \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ (p-1) & 0 & 0 & 0\end{pmatrix}\begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ r_3\end{pmatrix}. \tag{64}$$

Therefore we can easily write

$$(\mathcal{G}_k - \mathcal{G}_k^\dagger)\mathcal{L}_k^{m'-1}\begin{pmatrix} 1/2 \\ r_1 \\ r_2 \\ r_3\end{pmatrix} = i\begin{pmatrix} f(k,p,\vec{r}\,') \\ 0 \\ 0 \\ p-1\end{pmatrix}. \tag{65}$$

Now putting everything together, we get for the second moment $\langle x^2\rangle_t$

$$\langle x^2\rangle_t = (1-p)t + \int_{-\pi}^{\pi}\frac{dk}{\pi}\Gamma(k,p,t), \tag{66}$$

where (we drop out arguments for simplicity)

$$\Gamma = \sum_{m=1}^{t}\sum_{m'=1}^{m-1}\big(0\ (p-1)\ g\ h\big)\mathcal{L}_k^{m-m'-1}\begin{pmatrix} 0 \\ 0 \\ 0 \\ p-1\end{pmatrix}. \tag{67}$$

Note that the $f(k,p,\vec{r}')$ doesn't appear in Γ, since

$$\big(0\ (p-1)\ g\ h\big)\mathcal{L}_k^{m-m'-1}\begin{pmatrix} f(k,p,\vec{r}') \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0. \tag{68}$$

Same as before we can use the matrix M_k for calculating Eq. (67)

$$\Gamma = \big((p-1)\ g\ h\big)\left[\sum_{m=1}^{t}\sum_{m'=1}^{m-1} M_k^{m-m'-1}\right]\begin{pmatrix} 0 \\ 0 \\ p-1 \end{pmatrix}, \tag{69}$$

where

$$\begin{aligned}\sum_{m=1}^{t}\sum_{m'=1}^{m-1} M_k^{m-m'-1} &= (I-M_k)^{-1}\sum_{m=1}^{t}\big(I-M_k^m\big) \\ &= (I-M_k)^{-1}\{t-(I-M_k)^{-1}M\}. \end{aligned}\tag{70}$$

By inserting this into Eq. (69), the calculation of $\langle x^2\rangle_t$ will be straightforward.

Our interest is finding D here, so only the time-dependent terms will be important for us. By inserting the time dependent term of Eq. (70) into Eq. (66) and definition of D given in Eq. (59), we have

$$\begin{aligned} D &= \frac{1}{2}\lim_{t\to\infty}\frac{\partial\sigma^2}{\partial t} \\ &= \frac{1}{2}\left\{(1-p)+\int_{-\pi}^{\pi}\frac{dk}{\pi}\frac{\partial\Gamma}{\partial t}\right\}. \end{aligned}\tag{71}$$

The matrix $(I-M_k)^{-1}$ is exactly invertible but its elements are a little long to appears here. Fortunately, this matrix appears in the form of

$$\frac{\partial\Gamma}{\partial t} = \big((p-1)\ g\ h\big)(I-M_k)^{-1}\begin{pmatrix} 0 \\ 0 \\ p-1 \end{pmatrix}, \tag{72}$$

i.e., it is sandwiched between two vectors. It is not difficult to calculate Eq. (71) to have

$$\begin{aligned} D &= \frac{1}{2}\left\{(1-p)+\frac{(1-p)^2}{p}[1-I(1-p)]\right\} \\ &= \frac{1-p}{p}K(p), \end{aligned}\tag{73}$$

where

$$K(p) = \tfrac{1}{2}\{1-(1-p)I(1-p)\} \tag{74}$$

and

$$I(x) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{\cos(k)+x}{\cos(k)^2x+\cos(k)x+2x^2-2x+1}. \tag{75}$$

The expression of $D(p)$ in Eq. (73) is exactly same as the numerical result of Ref. [42] in which the authors have proposed a constant value for K and have estimated $K\approx 0.4$ by linear regression. But our analytical calculations show that the coefficient K is a function of p [Eq. (74)] and ranges from 0.19 to 0.5 as p goes from 0 to 1 (see Fig. 2). The numeric prediction of Romanelli *et al.* implies that for $p=0.44$ the diffusion coefficient is exactly the same as the unbiased classical random walk, i.e., 1/2, but our analytical calculations

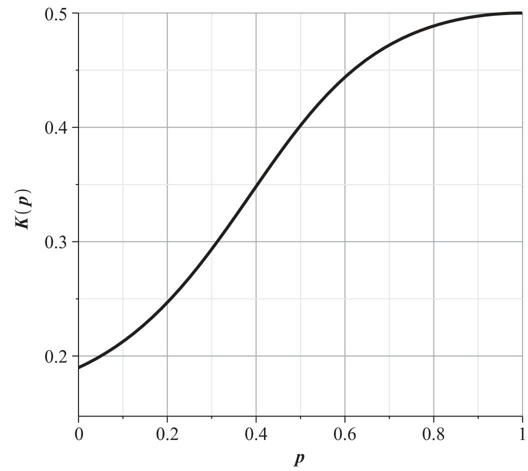

FIG. 2. The $K(p)$ versus p.

indicate that this probability is less than the numeric prediction and is about $p=0.417$. This means that for $p<0.417$ the diffusion coefficient is greater than the classical one and the quantum walker spreads more faster than the classical one. The origin of this difference is behind of the fact that the numerical method can never be applied in problems with infinite steps.

B. Coin decoherence

In this subsection we show that in the coin decoherence, the general formalism of Eq. (37) reduces to the formalism of Brun *et al.* presented in Ref. [39].

Let us suppose that before each step of walking, the operators $D_c^{(n)}$ acts on the coin subspace with probability p_n. Then according to Eq. (13) the A_n are

$$A_n = S(I\otimes H)\big(I\otimes D_c^{(n)}\big) = S\big(I\otimes HD_c^{(n)}\big). \tag{76}$$

By plugging it into Eq. (14) and using the explicit form of S we get

$$\begin{aligned} E_n = \sqrt{p_n}\sum_x &|x+1\rangle\langle x|\otimes|R\rangle\langle R|HD_c^{(n)} \\ &+|x-1\rangle\langle x|\otimes|L\rangle\langle L|HD_c^{(n)}. \end{aligned}\tag{77}$$

Now by writing the operator $HD_c^{(n)}$ in the basis $\{|R\rangle,|L\rangle\}$

$$HD_c^{(n)} = \sum_{r,s=\{R,L\}}\gamma_{r,s}^{(n)}|r\rangle\langle s| \tag{78}$$

the Eq. (77) takes the following form

$$\begin{aligned} E_n = \sqrt{p_n}\sum_x\sum_{s=\{R,L\}} &\gamma_{R,s}^{(n)}|x+1\rangle\langle x|\otimes|R\rangle\langle s| \\ &+\gamma_{L,s}^{(n)}|x-1\rangle\langle x|\otimes|L\rangle\langle s|. \end{aligned}\tag{79}$$

This equation is exactly in the form of Eq. (11) with the specified values for l, i.e., $l=1,-1$, hence

$$a_{1,R,s}^{(n)} = \gamma_{R,s}^{(n)}, \quad a_{-1,L,s}^{(n)} = \gamma_{L,s}^{(n)}. \tag{80}$$

Therefore according to Eq. (21) we have

$$C_n(k) = \sum_{j=\{L,R\}}\gamma_{R,j}^{(n)}e^{-ik}|R\rangle\langle j| + \gamma_{L,j}^{(n)}e^{ik}|L\rangle\langle j| \tag{81}$$

and

$$\frac{dC_n(k)}{dk} = -i \sum_{j=\{L,R\}} \gamma_{R,j}^{(n)} e^{-ik} |R\rangle\langle j| - \gamma_{L,j}^{(n)} e^{ik} |L\rangle\langle j| = -iZC_n(k). \tag{82}$$

And finally according to the definition of $\mathcal{L}_{k,k'}$ in Eq. (36)

$$\mathcal{G}_{k,k'}\tilde{O} = -iZ(\mathcal{L}_{k,k'}\tilde{O}). \tag{83}$$

Clearly $\mathcal{G}^{\dagger}_{k,k'}\tilde{O} = i(\mathcal{L}_{k,k'}\tilde{O})Z$, and the $\mathcal{J}_k$ in Eq. (38) will be

$$\mathcal{J}_k\tilde{O} = \left.\frac{d\mathcal{G}^{\dagger}_{k,k'}\tilde{O}}{dk}\right|_{k'=k} = Z(\mathcal{L}_k\tilde{O})Z. \tag{84}$$

Inserting Eq. (84) into the last term of Eq. (37) we get

$$\begin{aligned}
&\int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{m=1}^{t} \mathrm{Tr}\big\{\mathcal{J}_k\big(\mathcal{L}_k^{m-1}|\psi_0\rangle\langle\psi_0|\big)\big\} \\
&= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{m=1}^{t} \mathrm{Tr}\big\{Z\big[\mathcal{L}_k\big(\mathcal{L}_k^{m-1}|\psi_0\rangle\langle\psi_0|\big)\big]Z\big\} \\
&= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{m=1}^{t} \mathrm{Tr}\big\{\mathcal{L}_k^{m}|\psi_0\rangle\langle\psi_0|\big\} = t.
\end{aligned} \tag{85}$$

Finally, putting Eqs. (83) and (85) in the moment expressions of Eq. (37), reduces them to the same expression as introduced by Brun *et al.* [39] for only coin decoherence, i.e.,

$$\begin{aligned}
\langle x\rangle_t &= \int_{-\pi}^{\pi} \sum_{m=1}^{t} \frac{dk}{2\pi} \mathrm{Tr}\big\{Z\mathcal{L}_k^{m}|\psi_0\rangle\langle\psi_0|\big\} \\
\langle x^2\rangle_t &= t + \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{m=1}^{t}\sum_{m'=1}^{m-1} \mathrm{Tr}\big\{Z\mathcal{L}_k^{m-m'}\big(Z\mathcal{L}_k^{m'}|\psi_0\rangle\langle\psi_0|\big)\big\} \\
&\quad + \mathrm{Tr}\big\{Z\mathcal{L}_k^{m-m'}\big(\big(\mathcal{L}_k^{m'}|\psi_0\rangle\langle\psi_0|\big)Z\big)\big\}.
\end{aligned} \tag{86}$$

Therefor the first and second moments given in Eq. (37) are general in the sense that they can be applied for any types of decoherence, including coin-position decoherence, coin decoherence, and position decoherence.

V. SUMMARY AND CONCLUSION

We have presented an analytical method for calculating the first and second moments of the one-dimensional QW, which are applicable for all kinds of decoherence. Our method is a generalization of the Brun *et al.* method, introduced in Ref. [39], where there the authors have presented the analytical expressions for the first and second moments in the presence of coin decoherence and have shown that the transition from quantum to classic happens even for the weak coin noise.

We have made exact calculations on the broken line decoherence as an example of the nonseparable decoherence of the coin-position system. Our analytical calculations are inconsistent with the previous numerical result [42]. We have shown that the K in the diffusion coefficient D is, indeed, a function of p and ranges from 0.19 to 0.5 as p varies from 0 to 1.

Furthermore, our calculation shows that for $p = 0.417$ the value of D is $1/2$, exactly the same as the unbiased classical random walk. This specific value of p is critical in the sense that the transition from quantum to classic happens at this point. In other words, the quantum walk with nonzero broken line probability spreads faster than the classical random walk if the probability of broken line is not higher than 0.417. For higher values of p, the lines are broken too frequently and this will prevent the full diffusion. The critical p, estimated by the numerical calculation of Ref. [42], is a little higher than the one obtained here analytically. The difference arises from the nonability of numerical method in simulation of the QW with infinite steps. We have also studied the case that only the coin is subjected to decoherence and have shown that the expressions for the first and second moments lead to the Brun *et al.* results presented in Ref. [39].

The long time behavior of moments and, of course, the variance can be used as a qualitative measure of classicality. Therefore these calculated moments provides a powerful tool for investigating the one-dimensional QW in the presence of any kinds of decoherence. For instance, finding the particular cases for which dependency of the variance on the time remains quadratic, i.e., the decoherence does not affect the quantumness, is an application of these moments. Brun *et al.* [39] have shown that the quadratic time dependency of the variance is preserved for many-coins QW subjected to the coin decoherence, but their calculation is restricted to the coin decoherence only. In this article this restriction is relaxed and the model allows the presence of any kind of decoherence.

These formulas are useful also in the experimental implementation of the quantum walk. The application of our results for two kinds of decoherence, i.e., the coin-only and the coin-position noises, has been done in this article. The application on the position decoherence has been also tested but the full calculations were so long to appear here. The results of our calculations on the tunneling effect, for which the position is subjected to decoherence, and its consistency with the previous numerical work [33] confirm the usefulness of these expressions for the position decoherence too. Other aspects of the tunneling effects are also under consideration. The article, therefore, can be regarded as a further development in the study of decoherent one-dimensional QW.

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