Quantum walk on orbit spaces

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Inspired by the covering-space method in path integrals on multiply connected spaces, we here present a universal formula of time-evolution kernels for continuous- and discrete-time quantum walks on orbit spaces. In this note, we focus on the case in which walkers' configuration space is the orbit space Λ/Γ , where Λ is an arbitrary lattice and Γ is a discrete group whose action on Λ has no fixed points. We show that the time-evolution kernel on Λ/Γ can be written as a weighted sum of time-evolution kernels on Λ , where the summation is over the orbit of initial point in Λ and weight factors are given by a one-dimensional unitary representation of Γ . Focusing on one dimension, we present a number of examples of the formula. We also present universal formulas of resolvent kernels, canonical density matrices, and unitary representations of arbitrary groups in quantum walks on Λ/Γ , all of which are constructed in exactly the same way as for the time-evolution kernel.

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I. INTRODUCTION

Quantum walk-a quantum-mechanical analog of classical random walk on lattices or graphs-has been the subject of intense study over the last two decades. Just as in classical random walk, there exist two distinct formulations in quantum walk: continuous-time quantum walk and discrete-time quantum walk; the former is equivalent to tight-binding models in condensed matter physics, while the latter is a natural generalization of classical random walk and formulated without recourse to Hamiltonian operators. These two formulations have their own merits and their applications now appear in many disciplines, including the quantum search algorithm [1,2], universal quantum computation [3–6], and topological phases of matter [7]; see Refs. [8–10] for reviews. In both formulations, the central object is the probability amplitude for finding particles (walkers), which is given by a matrix element of the time-evolution operator in position space-the time-evolution kernel.¹ This time-evolution kernel is normally calculated through spectral decomposition or numerical calculation, which becomes harder as the matrix size becomes larger. It would therefore be desirable if a simpler method existed.

The purpose of this note is to present such a method by generalizing the Dowker's covering-space method [11] in path integral (see also Refs. [12–16]). As is well known, in quantum mechanics on continuous spaces, the time-evolution kernel can be represented by the Feynman path integral, which provides a number of powerful methods to analyze quantum systems nonperturbatively. Among them is the covering-space method: it provides a universal method to construct the timeevolution kernel on multiply connected spaces of the form $\mathcal{M} = \mathcal{M} / \pi_1(\mathcal{M})$, where \mathcal{M} is the universal covering space of \mathcal{M} and $\pi_1(\mathcal{M})$ is the fundamental group of \mathcal{M} . In this method, the path integral on \mathcal{M} is given by a linear combination of partial amplitudes, where each partial amplitude is given by the path integral on the universal covering space \mathcal{M} and linear-combination coefficients are given by onedimensional unitary representations of the fundamental group $\pi_1(\mathcal{M})$. Inspired by this method, we here present a universal formula for the time-evolution kernel in both continuous- and discrete-time quantum walks where walkers' configuration space can be regarded as the *orbit space* Λ/Γ . Here Λ is an arbitrary lattice and Γ is a discrete group whose action on Λ has no fixed points. A typical example for such configuration spaces is that for a single walker on a periodic lattice. Another typical example is the configuration space for identical walkers on an arbitrary lattice, where the indistinguishability of identical particles makes their configuration space an orbit space [13,17-20]. We show that the time-evolution kernel on the orbit space Λ/Γ can be written as a weighted sum of time-evolution kernels on Λ , where the summation is over the orbit of initial point in Λ and weight factors are given by a one-dimensional unitary representation of Γ . This universal formula offers a simpler method to construct the time-evolution kernel on Λ/Γ because computation becomes generally much easier on Λ .

In what follows, we first set up the problem and then present our main formula and its proof. We then present a number of examples of the formula in Sec. III. In Sec. IV, we present several other quantities that can be constructed in exactly the same way as for the time-evolution kernel. Examples include the resolvent kernel, the canonical density matrix, and a unitary representation of arbitrary groups. Section V is devoted to the conclusion. Appendix presents some sample computations in continuous-time quantum walk.

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¹The term "kernel" is a remnant of continuum theory. In quantum mechanics on continuous spaces, a matrix element of the time-evolution operator is given by an integral kernel.

Throughout this note we will use the units in which $\hbar = a = 1$, where *a* is a lattice spacing.

II. TIME-EVOLUTION KERNEL

To begin with, let us fix some notation. Let Λ be an arbitrary lattice (i.e., a discrete space spanned by a set of linearly independent vectors in a Euclidean space) and let Γ be a discrete group whose action on Λ has no fixed points. We note that Γ must be a discrete subgroup of the isometry of the Euclidean space, which consists of reflections, translations, and rotations. Let Λ/Γ be the orbit space (quotient space) given by the identification $x \sim \gamma x$ in Λ , where γx stands for the action of $\gamma \in \Gamma$ on $x \in \Lambda$ that satisfies the compatibility condition $\gamma_1(\gamma_2 x) = (\gamma_1 \gamma_2) x$ for any $\gamma_1, \gamma_2 \in \Gamma$ and $x \in \Lambda$. For the moment, we shall consider continuous-time quantum walk on the lattice Λ/Γ , where the Hilbert space \mathscr{H} is the set of square-summable sequences on Λ/Γ , $\mathscr{H} = l^2(\Lambda/\Gamma)$. (Note, however, that the formula presented below is turned out to be applicable to discrete-time quantum walk as well; see Sec. IV C.) The action of the time-evolution operator U_{τ} on a state $\psi_0 \in \mathscr{H}$ is defined by

$$(U_{\tau}\psi_0)(x) := \sum_{y \in \Lambda/\Gamma} U_{\tau}(x, y)\psi_0(y), \quad \forall x \in \Lambda/\Gamma, \quad (1)$$

where $U_{\tau}(x, y)$ is the time-evolution kernel and the subscript $\tau \in \mathbb{R}$ represents the time. The probability for finding a particle at the time τ and at the position *x* is then given by

$$P_{\tau}(x) = |(U_{\tau}\psi_0)(x)|^2.$$
(2)

In particular, if the particle is initially localized at $x = x_0$ [i.e., $\psi_0(x) = \delta_{x,x_0}$], the probability is simply given by $P_{\tau}(x) = |U_{\tau}(x,x_0)|^2$.

In the following, we shall construct $U_{\tau}(x, y)$ in terms of the time-evolution kernel on Λ . The key is the group property of the time-evolution operator.

A. The formula

The time-evolution operator U_{τ} is a one-parameter family of unitary operators. It satisfies the composition law $U_{\tau_1}U_{\tau_2} = U_{\tau_1+\tau_2}$, the unitarity $U_{\tau}^{\dagger}(=U_{\tau}^{-1}) = U_{-\tau}$, and the initial condition $U_0 = I$, where *I* stands for the identity operator. Correspondingly, the time-evolution kernel $U_{\tau}(\cdot, \cdot)$ must satisfy the following properties:

(1) Property 1 (Composition law):

$$\sum_{z \in \Lambda/\Gamma} U_{\tau_1}(x, z) U_{\tau_2}(z, y) = U_{\tau_1 + \tau_2}(x, y), \quad \forall x, y \in \Lambda/\Gamma.$$

$$\overline{U_{\tau}(x, y)} = U_{-\tau}(y, x), \quad \forall x, y \in \Lambda/\Gamma.$$
(3b)

(3) Property 3 (Initial condition):

(2) Property 2 (Unitarity):

$$U_0(x, y) = \delta_{x, y}, \quad \forall x, y \in \Lambda / \Gamma.$$
 (3c)

Here the overline $(\overline{})$ stands for the complex conjugate. As we shall prove shortly, such a kernel can be constructed as

follows:

$$U_{\tau}(x, y) = \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{\tau}(x, \gamma y), \qquad (4)$$

where $D: \Gamma \to U(1)$ $(\gamma \mapsto D(\gamma))$ is a one-dimensional unitary representation of Γ that satisfies the group composition law $D(\gamma)D(\gamma') = D(\gamma\gamma')$ and the unitarity $\overline{D(\gamma)} = D$ $(\gamma)^{-1} = D(\gamma^{-1})$ for any $\gamma, \gamma' \in \Gamma$. Here $\widetilde{U}_{\tau}(\cdot, \cdot)$ is a timeevolution kernel on Λ that satisfies the following assumptions:

(1) Assumption 1 (Composition law):

$$\sum_{z \in \Lambda} \widetilde{U}_{\tau_1}(x, z) \widetilde{U}_{\tau_2}(z, y) = \widetilde{U}_{\tau_1 + \tau_2}(x, y), \quad \forall x, y \in \Lambda.$$
(5a)

$$\overline{\widetilde{U}_{\tau}(x,y)} = \widetilde{U}_{-\tau}(y,x), \quad \forall x, y \in \Lambda.$$
(5b)

(3) Assumption 3 (Initial condition):

$$U_0(x, y) = \delta_{x,y}, \quad \forall x, y \in \Lambda.$$
 (5c)

(4) Assumption 4 (Γ invariance):

$$\widetilde{U}_{\tau}(\gamma x, \gamma y) = \widetilde{U}_{\tau}(x, y), \quad \forall x, y \in \Lambda, \quad \forall \gamma \in \Gamma.$$
(5d)

We note that the Γ invariance (5d) is guaranteed if the Hamiltonian operator on Λ is invariant under the action of Γ .

Before giving the proof, let us first present a quick derivation of formula (4) by following the Dowker method [11]. To this end, let $\tilde{\psi}_{\tau}(x)$ be an equivariant function on Λ that satisfies $\tilde{\psi}_{\tau}(\gamma x) = D(\gamma)\tilde{\psi}_{\tau}(x)$ for any $x \in \Lambda$ and $\gamma \in \Gamma$. (The reason for using this will be apparent shortly.) Then we have

$$\begin{split} \widetilde{\psi}_{\tau}(x) &= \sum_{y \in \Lambda} \widetilde{U}_{\tau}(x, y) \widetilde{\psi}_{0}(y) \\ &= \sum_{y \in \Lambda/\Gamma} \sum_{\gamma \in \Gamma} \widetilde{U}_{\tau}(x, \gamma y) \widetilde{\psi}_{0}(\gamma y) \\ &= \sum_{y \in \Lambda/\Gamma} \sum_{\gamma \in \Gamma} \widetilde{U}_{\tau}(x, \gamma y) D(\gamma) \widetilde{\psi}_{0}(y) \\ &= \sum_{y \in \Lambda/\Gamma} \left(\sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{\tau}(x, \gamma y) \right) \widetilde{\psi}_{0}(y), \end{split}$$
(6)

where in the second equality we have used the following identity:

$$\sum_{x \in \Lambda} f(x) = \sum_{x \in \Lambda/\Gamma} \sum_{\gamma \in \Gamma} f(\gamma x).$$
(7)

Here f(x) is an arbitrary test function on Λ . This identity just says that first summing over the orbit $\Gamma \cdot x := \{\gamma x : \gamma \in \Gamma\}$ of $x \in \Lambda/\Gamma$ and then summing over all $x \in \Lambda/\Gamma$ yields the summation over the whole space Λ . By comparing Eq. (6) with definition (1), we arrive at formula (4).

Now, since $U_{\tau}(\cdot, \cdot)$ is defined on the lattice Λ , the domain of $U_{\tau}(\cdot, \cdot)$ defined by Eq. (4) can be naturally extended from Λ/Γ to Λ . In particular, it satisfies the following equation:

$$U_{\tau}(\gamma x, y) = D(\gamma)U_{\tau}(x, y), \quad \forall x, y \in \Lambda, \quad \forall \gamma \in \Gamma.$$
(8)

(3a)

In fact, a straightforward calculation gives

$$\begin{aligned} U_{\tau}(\gamma x, y) &= \sum_{\gamma' \in \Gamma} D(\gamma') \widetilde{U}_{\tau}(\gamma x, \gamma' y) \\ &= \sum_{\gamma' \in \Gamma} D(\gamma \gamma^{-1} \gamma') \widetilde{U}_{\tau}(\gamma^{-1} \gamma x, \gamma^{-1} \gamma' y) \\ &= D(\gamma) \sum_{\gamma' \in \Gamma} D(\gamma^{-1} \gamma') \widetilde{U}_{\tau}(x, \gamma^{-1} \gamma' y) \\ &= D(\gamma) \sum_{\gamma'' \in \Gamma} D(\gamma'') \widetilde{U}_{\tau}(x, \gamma'' y) \\ &= D(\gamma) U_{\tau}(x, y), \end{aligned}$$
(9)

where the second equality follows from the Γ invariance (5d) and the third equality follows from the group composition law $D(\gamma\gamma^{-1}\gamma') = D(\gamma)D(\gamma^{-1}\gamma')$. In the fourth equality, we have changed the summation variable from γ' to $\gamma'' := \gamma^{-1}\gamma'$. It is now obvious from Eq. (8) that $(U_\tau\psi_0)(x)$ defined by Eq. (1) also satisfies $(U_\tau\psi_0)(\gamma x) = D(\gamma)(U_\tau\psi_0)(x)$ for any $x \in \Lambda$ and $\gamma \in \Gamma$; that is, $(U_\tau\psi_0)(x)$ becomes an equivariant function on Λ . This is the reason why we used the equivariant function in the above derivation. As we shall see in Sec. III, Eq. (8) provides boundary conditions on Λ/Γ .

Finally, let us comment on the case where the action of Γ has fixed points. First, identity (7) does not hold in general if there is a fixed point: if there is a point $x \in \Lambda$ that satisfies $\gamma x = x$ for some $\gamma \neq e \in \Gamma$, where e stands for the identity element of Γ , the right-hand side of Eq. (7) leads to an overcounting of the fixed point x^2 . Note, however, that if f(x) is subject to the Dirichlet boundary condition at the fixed point, such an overcounting does not occur so that Eq. (7) holds true even in the presence of fixed points.³ Note that the Dirichlet boundary condition f(x) = 0 at $x = \gamma x$ can be deduced from the equivariant property $D(\gamma)f(x) = f(\gamma x) =$ f(x) if $D(\gamma) \neq 1$. Hence, if $D: \Gamma \to U(1)$ is not the trivial representation, our formula (4) can be applied equally well to the case in which the action of Γ has fixed points. For the case of the trivial representation, however, the equivariant property does not lead to any definite boundary conditions. For simplicity, in this note we will mainly focus on the case where Γ has no fixed points.

B. Proof

Now we show that $U_{\tau}(\cdot, \cdot)$ given by formula (4) satisfies the required properties (3a)–(3c) if *D* is a one-dimensional unitary representation of Γ and if $\widetilde{U}_{\tau}(\cdot, \cdot)$ satisfies the assumptions (5a)–(5d). The proof is by direct computation. Each property is proved as follows. (See also Refs. [21–23] for similar proofs in path integral.)

Property 1 (Composition law). Let us first prove the composition law (3a). By substituting Eq. (4) into the left-hand

side of Eq. (3a), we get

$$\sum_{z \in \Lambda/\Gamma} U_{\tau_1}(x, z) U_{\tau_2}(z, y)$$

$$= \sum_{z \in \Lambda/\Gamma} \sum_{\gamma_1 \in \Gamma} \sum_{\gamma_2 \in \Gamma} D(\gamma_1) D(\gamma_2) \widetilde{U}_{\tau_1}(x, \gamma_1 z) \widetilde{U}_{\tau_2}(z, \gamma_2 y)$$

$$= \sum_{z \in \Lambda/\Gamma} \sum_{\gamma_1 \in \Gamma} \sum_{\gamma_2 \in \Gamma} D(\gamma_1 \gamma_2) \widetilde{U}_{\tau_1}(x, \gamma_1 z) \widetilde{U}_{\tau_2}(\gamma_1 z, \gamma_1 \gamma_2 y)$$

$$= \sum_{\gamma \in \Gamma} D(\gamma) \sum_{z \in \Lambda/\Gamma} \sum_{\gamma_1 \in \Gamma} \widetilde{U}_{\tau_1}(x, z) \widetilde{U}_{\tau_2}(z, \gamma y)$$

$$= \sum_{\gamma \in \Gamma} D(\gamma) \sum_{z \in \Lambda} \widetilde{U}_{\tau_1}(x, z) \widetilde{U}_{\tau_2}(z, \gamma y)$$

$$= \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{\tau_1 + \tau_2}(x, \gamma y)$$

$$= U_{\tau_1 + \tau_2}(x, y), \qquad (10)$$

where the second equality follows from the group composition law $D(\gamma_1)D(\gamma_2) = D(\gamma_1\gamma_2)$ and the Γ invariance (5d). The third equality follows from the change of the summation variable from γ_2 to $\gamma := \gamma_1\gamma_2$, and the fourth equality follows from formula (7). Finally, the fifth equality follows from assumption (5a).

Property 2 (Unitarity). Let us next prove unitarity (3b). By substituting Eq. (4) into the left-hand side of Eq. (3b), we get

$$\overline{U_{\tau}(x, y)} = \sum_{\gamma \in \Gamma} \overline{D(\gamma)} \, \overline{\widetilde{U}_{\tau}(x, \gamma y)}$$
$$= \sum_{\gamma \in \Gamma} D(\gamma^{-1}) \widetilde{U}_{-\tau}(\gamma y, x)$$
$$= \sum_{\gamma \in \Gamma} D(\gamma^{-1}) \widetilde{U}_{-\tau}(y, \gamma^{-1} x)$$
$$= U_{-\tau}(y, x),$$
(11)

where the second equality follows from the unitarity properties $\overline{D(\gamma)} = D(\gamma^{-1})$ and (5b). The third equality follows from the Γ invariance (5d), and the last equality follows from definition (4) (where the summation is over γ^{-1} instead of γ).

Property 3 (Initial condition). Let us finally prove the initial condition (3c). By substituting Eq. (4) into the left-hand side of Eq. (3c), we get

$$U_{0}(x, y) = \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{0}(x, \gamma y)$$

$$= \sum_{\gamma \in \Gamma} D(\gamma) \delta_{x, \gamma y}$$

$$= D(e) \delta_{x, ey}$$

$$= \delta_{x, y}, \qquad (12)$$

where the second equality follows from assumption (5c). The third equality follows from the fact that *x* and γy cannot be equal for any $x, y \in \Lambda/\Gamma$ except for the case $\gamma = e$. Finally, the last equality follows from D(e) = 1 for any one-dimensional unitary representations of Γ .

²In general, Eq. (7) becomes $\sum_{x \in \Lambda} f(x) = \sum_{x \in (\Lambda - \Delta)/\Gamma} \sum_{\gamma \in \Gamma} f(x) + \sum_{x \in \Delta} f(x)$, where Δ stands for the set of fixed points of Γ . ³More generally, such an overcounting does not occur if $\sum_{x \in \Delta} f(x) = 0$.

Putting all the above things together, we see that Eq. (4) is the sufficient condition to be the time-evolution kernel on the orbit space Λ/Γ . This completes the proof.

III. EXAMPLES

There exist a number of examples in which walkers' configuration space can be regarded as an orbit space. Typical examples are a single walker on a torus, the half space, and a cubic. Another typical example is identical walkers on an arbitrary lattice, where their configuration space always becomes an orbit space. In this section, we shall focus on one spatial dimension for simplicity and present several examples that fit into formula (4). Let us start with single-walker examples.

A. A single walker in one dimension

Let $\widetilde{U}_{\tau}(x, y)$ be a time-evolution kernel on the integer lattice $\Lambda = \mathbb{Z}$ that satisfies the composition law (5a), the unitarity (5b), and the initial condition (5c), as well as the translation invariance $\widetilde{U}_{\tau}(x + z, y + z) = \widetilde{U}_{\tau}(x, y)$ and the reflection invariance $\widetilde{U}_{\tau}(z - x, z - y) = \widetilde{U}_{\tau}(x, y)$ for any $x, y, z \in \mathbb{Z}$. A typical example of such a kernel is that of a free particle given by $\widetilde{U}_{\tau}(x, y) = e^{i\frac{\pi}{2}|x-y|}J_{|x-y|}(\omega\tau)$, where J_n is the Bessel function of the first kind and $\omega(> 0)$ is a hopping parameter; see Eq. (A8) in Appendix. [Note, however, that the formulas presented below are not limited to free-particle theories. They are robust against any perturbations unless boundary conditions (8) are changed.] Below we shall construct time-evolution kernels for a single walker on a circle, the half line, and a finite interval by gauging these discrete symmetries.

Example 1 (A single walker on a circle). Let us first consider a single walker on a periodic lattice of *L* sites, $\{1, 2, ..., L \pmod{L}\}$. This lattice can be constructed from \mathbb{Z} by making the identification $x \sim x + nL$, where *n* is an arbitrary integer; see Fig. 1(a). Hence, the configuration space is the orbit space $\mathbb{Z}/L\mathbb{Z}$, where $L\mathbb{Z} = \langle t | \emptyset \rangle$ is the free group generated by a translation *t*. Its action on \mathbb{Z} is defined by

$$tx := x + L. \tag{13}$$

Note that any element of $L\mathbb{Z}$ can be written as the product t^n , whose action on \mathbb{Z} is given by $t^n x = x + nL$.

Now we need to find out one-dimensional unitary representations of $L\mathbb{Z}$. Since $L\mathbb{Z}$ is the free group generated by a single generator *t*, we have a one-parameter family of maps $D^{[\theta]} : L\mathbb{Z} \to U(1)$ labeled by an angle parameter θ ,

$$D^{[\theta]}(t) = e^{i\theta}, \qquad (14)$$

where $\theta \in \mathbb{R}/2\pi\mathbb{R}$. It then follows from formula (4) that the time-evolution kernel for a single walker on $\mathbb{Z}/L\mathbb{Z}$ takes the following form:

$$U_{\tau}^{[\theta]}(x, y) = \sum_{n=-\infty}^{\infty} D^{[\theta]}(t^n) \widetilde{U}_{\tau}(x, t^n y)$$
$$= \sum_{n=-\infty}^{\infty} e^{in\theta} \widetilde{U}_{\tau}(x, y + nL).$$
(15)

Just as in the path integral on a circle (see, e.g., Sec. 2.4 of Ref. [24]), Eq. (15) represents the summation over winding

numbers. Physically, Eq. (15) describes the situation in which the walker acquires the Aharonov-Bohm phase $e^{i\theta}$ every time it winds around the circle, where θ plays the role of a magnetic flux penetrating through the circle. This is the physical meaning of the weight factor (14) and the summation over the orbit of initial point. See also Fig. 1(a).

Now two remarks are in order. First, it follows from Eq. (8) that $U_{\tau}^{[\theta]}(\cdot, \cdot)$ satisfies the identity $U_{\tau}^{[\theta]}(x + L, y) = e^{i\theta}U_{\tau}^{[\theta]}(x, y)$; that is, it satisfies the twisted boundary conditions $U_{\tau}^{[\theta]}(L + 1, y) = e^{i\theta}U_{\tau}^{[\theta]}(1, y)$ and $U_{\tau}^{[\theta]}(0, y) = e^{-i\theta}U_{\tau}^{[\theta]}(L, y)$. Namely, Eq. (15) gives the universal formula of the time-evolution kernel for a single walker on a circle subject to these twisted boundary conditions.

The second remark is that, under the reflection, Eq. (15) satisfies $U_{\tau}^{[\theta]}(z-x, z-y) = U_{\tau}^{[-\theta]}(x, y)$. Hence, at $\theta = 0$ or $\pi \pmod{2\pi}$, Eq. (15) becomes reflection invariant. We can use this invariance for the construction of time-evolution kernels on a finite interval; see example 3.

Example 2 (A single walker on the half line). Let us next consider a single walker on a semi-infinite lattice $\{1, 2, ...\}$. This lattice can be constructed from the integer lattice \mathbb{Z} by making the identification $x \sim 1 - x$; see Fig. 1(b). Hence, the configuration space is the orbit space \mathbb{Z}/\mathbb{Z}_2 , where $\mathbb{Z}_2 = \langle r | r^2 = e \rangle$ is the cyclic group of order 2. Here *r* is the reflection whose action on \mathbb{Z} is defined by

$$rx := 1 - x. \tag{16}$$

Note that $r^2x = x$. Note also that reflection (16) does not have a fixed point in the integer lattice. (Its fixed point is x = 1/2.)

Now, since $r^2 = e$, any one-dimensional unitary representation $D : \mathbb{Z}_2 \to U(1)$ must satisfy the condition $D(r)^2 = 1$, whose solution is $D(r) = \pm 1$. Hence, there exist two distinct maps $D^{[\phi]}$ given by

$$D^{[\phi]}(r) = \mathrm{e}^{i\phi},\tag{17}$$

where $\phi \in \{0, \pi \pmod{2\pi}\}$. Correspondingly, there exist the following two distinct time-evolution kernels for a single walker on \mathbb{Z}/\mathbb{Z}_2 :

$$U_{\tau}^{[\phi]}(x, y) = \sum_{n=0}^{1} D^{[\phi]}(r^{n}) \widetilde{U}_{\tau}(x, r^{n}y)$$

= $\widetilde{U}_{\tau}(x, y) + e^{i\phi} \widetilde{U}_{\tau}(x, 1-y).$ (18)

Again, just as in the path integral on the half line [21,25,26], Eq. (18) represents the summation over bouncing numbers off the boundary: the n = 0 term is the contribution from the direct path, while the n = 1 term is the contribution from the reflected path off the boundary. The physical meaning of the weight factor (17) is now clear: it plays the role of the reflection amplitude off the boundary. In other words, the walker acquires the phase shift ϕ when reflected from the boundary. See also Fig. 1(b).

Notice that Eq. (18) satisfies the identity $U_{\tau}^{[\phi]}(1-x, y) = e^{i\phi}U_{\tau}^{[\phi]}(x, y)$; that is, it satisfies the boundary condition $U_{\tau}^{[\phi]}(0, y) = e^{i\phi}U_{\tau}^{[\phi]}(1, y)$. Hence, Eq. (18) gives the universal form of the time-evolution kernel for a single walker on the half line subject to this boundary condition. We emphasize that, as noted at the end of Sec. II A, if one wants a theory subject to the Dirichlet boundary condition at x = 0, one



FIG. 1. Construction of one-dimensional orbit spaces $\mathbb{Z}/L\mathbb{Z}$, \mathbb{Z}/\mathbb{Z}_2 , and \mathbb{Z}/D_∞ and typical single-walker trajectories. In the space-time picture, these orbit spaces correspond to a cylinder, the half space, and a finite strip. (a) A cylinder of circumference *L* is constructed by rolling up the infinite strip. This is equivalent to making the identification $x \sim x + nL$ ($n = 0, \pm 1, \pm 2, ...$) in the infinite strip. Under this identification, a single-walker trajectory with the initial and final points y + nL and x is mapped to a trajectory that starts from the initial point y and reaches the final point x after winding around the cylinder n times in the clockwise direction. The walker acquires the Aharonov-Bohm phase $e^{i\theta}$ every time it winds around the cylinder, and this phase is described by the unitary representation $D^{[\theta]} : L\mathbb{Z} \to U(1)$. (b) The half space with the boundary at x = 1/2 is constructed by folding the infinite strip in half at x = 1/2. This is equivalent to making the identification $x \sim 1 - x$ in the infinite strip. (Note, however, that noninteger points are excluded in the integer lattice. Hence, the boundary is in fact at x = 1 in our lattice problem.) Under this identification, a single-walker trajectory with the initial and final points 1 - y and x is mapped to a trajectory that bounces off the boundary. The walker acquires the phase $e^{i\phi} = \pm 1$ every time it hits the boundary, and this phase is described by the unitary representation $D^{[\phi]} : \mathbb{Z}_2 \to U(1)$. (c) A finite strip with the boundaries at x = 1/2 and 1/2 + L is constructed by folding up the infinite strip. Under these identifications, a single-particle trajectory with the initial and final points y - 2nL and $x \sim 1 - x + 2nL$ in the infinite strip. Under these identifications, a single-particle trajectory with the initial and final points y - 2nL (1 - y + 2nL) and x is mapped to a trajectory that bounces off the boundaries 2n (2n + 1) times. The walker acquires

should consider the reflection defined by rx := -x and choose the representation $\phi = \pi$. In this case, one arrives at the formula $U_{\tau}^{[\phi=\pi]}(x, y) = \widetilde{U}_{\tau}(x, y) - \widetilde{U}_{\tau}(x, -y)$ which satisfies $U_{\tau}^{[\phi=\pi]}(0, y) = 0$.

Example 3 (A single walker on a finite interval). Let us next consider a single walker on a finite interval of L sites, $\{1, 2, ..., L\}$. This lattice can be constructed from \mathbb{Z} by making the identifications $x \sim x + 2nL$ and $x \sim 1 - x + 2nL$, where n is an arbitrary integer; see Fig. 1(c). Hence, the configuration space is the orbit space \mathbb{Z}/D_{∞} , where $D_{\infty} = \mathbb{Z} \rtimes \mathbb{Z}_2 = \langle t, r | r^2 = e, rtr = t^{-1} \rangle$ is the infinite dihedral group generated by a translation t and a reflection

r.⁴ The actions of these operators on \mathbb{Z} are defined as follows:

$$tx := x + 2L$$
 and $rx := 1 - x$. (19)

Note that any element of D_{∞} can be written as $t^n r^m$, where $n = 0, \pm 1, \pm 2, \ldots$ and m = 0, 1. The action of this operator on \mathbb{Z} is given by $t^n r^m x = x + 2nL$ for m = 0 and

⁴The infinite dihedral group can also be written as the free product $D_{\infty} \cong \mathbb{Z}_2 * \mathbb{Z}_2 = \langle r, r' | r^2 = e, r'^2 = e \rangle$, where r'(=tr) is another reflection defined by r'x := 2L + 1 - x.

 $t^n r^m x = 1 - x + 2nL$ for m = 1, respectively. Note also that, in contrast to the previous examples, D_{∞} is a non-Abelian discrete group.

Now, since $r^2 = e$ and $rtr = t^{-1}$, any one-dimensional unitary representation $D: D_{\infty} \to U(1)$ must satisfy the conditions $D(r)^2 = 1$ and $D(r)D(t)D(r) = D(t)^{-1}$, which leads to $D(t)^2 = 1$. Thus, we have $D(t) = \pm 1$ and $D(r) = \pm 1$; that is, there exist $2^2 = 4$ distinct maps $D^{[\theta,\phi]}$ given by

$$D^{[\theta,\phi]}(t) = e^{i\theta}$$
 and $D^{[\theta,\phi]}(r) = e^{i\phi}$, (20)

where $\theta, \phi \in \{0, \pi \pmod{2\pi}\}$. Correspondingly, there exist the following four distinct time-evolution kernels for a single walker on \mathbb{Z}/D_{∞} :

$$U_{\tau}^{[\theta,\phi]}(x,y) = \sum_{n=-\infty}^{\infty} \sum_{m=0}^{1} D^{[\theta,\phi]}(t^{n}r^{m}) \widetilde{U}_{\tau}(x,t^{n}r^{m}y)$$
$$= \sum_{n=-\infty}^{\infty} [e^{in\theta} \widetilde{U}_{\tau}(x,y+2nL)$$
$$+ e^{in\theta} e^{i\phi} \widetilde{U}_{\tau}(x,1-y+2nL)].$$
(21)

Once again, just as in the path integral on a finite interval [22,27–29], Eq. (21) represents the summation over bouncing numbers off the two boundaries. Physically, $e^{i\phi}$ and $e^{i(\theta+\phi)}$ play the roles of the reflection amplitudes off the boundaries x = 1 and x = L, respectively. See also Fig. 1(c).

Now, it follows from Eq. (8) that Eq. (21) satisfies the identities $U_{\tau}^{[\theta,\phi]}(x+2L, y) = e^{i\theta}U_{\tau}^{[\theta,\phi]}(x, y)$ and $U_{\tau}^{[\theta,\phi]}(1-x, y) = e^{i\phi}U_{\tau}^{[\theta,\phi]}(x, y)$, which implies the boundary conditions $U_{\tau}^{[\theta,\phi]}(0, y) = e^{i\phi}U_{\tau}^{[\theta,\phi]}(1, y)$ and $U_{\tau}^{[\theta,\phi]}(L+1, y) = e^{i(\theta+\phi)}U_{\tau}^{[\theta,\phi]}(L, y)$. This means that Eq. (21) gives the universal form of the time-evolution kernel for a single walker on the finite interval subject to these boundary conditions. If one wants a theory that satisfies the Dirichlet boundary conditions at x = 0 and x = L + 1, one should redefine the translation and reflection as tx := x + 2(L+1) and rx := -x, respectively, and choose the representation $\phi = \pi$. In this case, one obtains

$$U_{\tau}^{[\theta,\phi=\pi]}(x,y) = \sum_{n=-\infty}^{\infty} e^{in\theta} \{ \widetilde{U}_{\tau}(x,y+2n(L+1)) - \widetilde{U}_{\tau}(x,-y+2n(L+1)) \},$$

which satisfies $U_{\tau}^{[\theta,\phi=\pi]}(0,y) = 0$ and $U_{\tau}^{[\theta,\phi=\pi]}(L+1,y) = 0$.

We note in closing that Eq. (21) can also be obtained from the time-evolution kernel on a circle (15) by gauging the reflection invariance at $\theta = 0$, $\pi \pmod{2\pi}$. In fact, Eq. (21) can be written as

$$U_{\tau}^{[\theta,\phi]}(x,y) = \sum_{m=0}^{1} D^{[\phi]}(r^m) U_{\tau}^{[\theta]}(x,r^m y)$$
$$= \sum_{m=0}^{1} \sum_{n=-\infty}^{\infty} D^{[\phi]}(r^m) D^{[\theta]}(t^n) \widetilde{U}_{\tau}(x,t^n r^m y),$$

where $D^{[\phi]}$ is the one-dimensional unitary representation of \mathbb{Z}_2 given by Eq. (17). An important lesson from this example is that there could exist several ways to construct time-evolution kernels on orbit spaces.

B. Identical walkers in one dimension

Now let us turn to the problem of multiple identical walkers on a lattice. The key to this problem is the *indistinguishability* of identical particles, where physical observables must be invariant under permutations of multiparticle coordinates. As is well known, this indistinguishability always makes the multiparticle configuration space an orbit space [13,17–20]. The basic idea behind this is to regard the permutation invariance as a *gauge symmetry* (i.e., redundancy in description). From this perspective, the configuration space must be a collection of inequivalent gauge orbits because gauge-equivalent configurations are physically equivalent.

To date, there exist two distinct formulations of this idea in identical-particle problems. The first regards the configuration space of N identical particles as the orbit space $(X^N - \Delta_N)/S_N$, where X^N is the N-fold Cartesian product of a single-particle configuration space X and $\Delta_N \subset X^N$ is the set of fixed points under the action of the symmetric group S_N [13,17–19]. On the other hand, the second includes the fixed points and regards the configuration space as the orbit space X^N/S_N [20]. The difference between these two formulations is very subtle (especially in lattices) and beyond the scope of this note. Fortunately, however, we can circumvent this issue and solve the N-identical-walker problems as follows.

Suppose that X itself is a nontrivial orbit space and takes the form $X = \widetilde{X}/G$, where G is a discrete group whose action on \widetilde{X} has no fixed points. In this case, the configuration space can also be written as $(\widetilde{X}^N - \widetilde{\Delta}_N)/(G \wr S_N)$ or $\widetilde{X}^N/(G \wr S_N)$.⁵ Here \wr stands for the wreath product defined by the semidirect product $G \wr S_N := G^N \rtimes S_N$ and $\widetilde{\Delta}_N \subset \widetilde{X}^N$ is the set of fixed points of S_N . Hence, irrespective of the formulations, once given a time-evolution kernel on $\Lambda = \widetilde{X}^N - \widetilde{\Delta}_N$ or \widetilde{X}^N , the problem just reduces to the classification of one-dimensional unitary representations of the discrete group $\Gamma = G \wr S_N$.

In this section, we shall focus on the cases $X = \mathbb{Z}$, $\mathbb{Z}/L\mathbb{Z}$, \mathbb{Z}/\mathbb{Z}_2 , and \mathbb{Z}/D_{∞} and construct time-evolution kernels for *N* identical walkers on the infinite line, a circle, the half line, and a finite interval. In the following, $\widetilde{U}_{\tau}(x, y)$ represents a time-evolution kernel on $\mathbb{Z}^N - \widetilde{\Delta}_N$ or \mathbb{Z}^N that satisfies the translation invariance, reflection invariance, and permutation invariance.

⁵Here is the proof. First, the wreath product $G \wr S_N = G^N \rtimes S_N$ can be written as the set $\{g\sigma : g \in G^N, \sigma \in S_N\}$ equipped with the group composition law $(g\sigma)(g'\sigma') = (g\sigma g'\sigma^{-1})(\sigma\sigma')$ for any $g, g' \in G^N$ and $\sigma, \sigma' \in S_N$. Here $g \mapsto \sigma g\sigma^{-1}$ is the automorphism of the *N*fold direct-product group $G^N = G \times \cdots \times G$ defined by $\sigma g\sigma^{-1} :=$ $g_{\sigma(1)} \dots g_{\sigma(N)}$ for any $g = g_1 \dots g_N \in G \times \cdots \times G$. It is now obvious that first making the identification $x \sim gx$ by $g \in G^N$ in \widetilde{X}^N and then making the identification $x \sim \sigma gx$ by $\sigma g = (\sigma g\sigma^{-1})\sigma \in G \wr S_N$ in \widetilde{X}^N . Hence, $(\widetilde{X}^N/G^N)/S_N$ is equivalent to $\widetilde{X}^N/(G \wr S_N)$. By subtracting the set of fixed points of S_N , we also see that $(\widetilde{X}^N/G^N - \Delta_N)/S_N$ is equivalent to $(\widetilde{X}^N - \widetilde{\Delta}_N)/(G \wr S_N)$. See also Refs. [20,30] for similar results in continuous spaces.



FIG. 2. Typical time evolutions of two identical particles on the infinite line with the initial and final points $y = (y_1, y_2)$ and $x = (x_1, x_2)$. When N = 2, the time-evolution kernel (25) consists of only two terms, $U_{\tau}^{[\pm]}(x_1, x_2, y_1, y_2) = \widetilde{U}_{\tau}(x_1, x_2, y_1, y_2) \pm$ $U_{\tau}(x_1, x_2, y_2, y_1)$. In the space-time picture, the first and second terms correspond to time evolutions of two identical particles without and with particle exchange, respectively; see the left panels. In the configuration-space picture, on the other hand, these terms correspond to a direct and reflected paths; see the right panels. In the latter picture, the particle-exchange phase ± 1 is described by the phase shift by reflecting off the boundary. [Note that the two-particle configuration space is the two-dimensional lattice with the identification $(x_1, x_2) \sim (x_2, x_1)$, which has the boundary at $x_1 = x_2$ and is identical to the half space ($\mathbb{Z}^2 - \Delta_2$)/ $S_2 \cong \{(x_1, x_2) \in \mathbb{Z}^2 : x_1 < x_2\}$ or $\mathbb{Z}^2/S_2 \cong \{(x_1, x_2) \in \mathbb{Z}^2 : x_1 \leqslant x_2\}$.]

Example 4 (N identical walkers on the infinite line). Let us first consider *N* identical walkers on the integer lattice \mathbb{Z} . In this case, the discrete group $\Gamma = S_N$ is just the symmetric group of order *N*!, whose presentation is

$$S_N = \langle \sigma_1, \dots, \sigma_{N-1} | \sigma_i^2 = e, \ \sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}, \sigma_i \sigma_j = \sigma_j \sigma_i \ (|i-j| \ge 2) \rangle.$$
(22)

Here $\sigma_i = (i, i + 1)$ is the adjacent transposition that interchanges *i* and *i* + 1. Its action on $x = (x_1, \ldots, x_N) \in \mathbb{Z}^N$ is defined as follows:

$$\sigma_i x := (x_1, \dots, x_{i-1}, x_{i+1}, x_i, x_{i+2}, \dots, x_N).$$
(23)

An arbitrary element $\sigma \in S_N$ can be written as a product of the generators $\sigma_1, \ldots, \sigma_{N-1}$. Its action on $x = (x_1, \ldots, x_N)$ can be written as $\sigma x = (x_{\sigma(1)}, \ldots, x_{\sigma(N)})$, where $\sigma(i)$ stands for the permutation of *i* under σ .

Now, there exist two distinct one-dimensional unitary representations of S_N : the trivial representation and the sign representation. Though this result is well known, let us reproduce it here just for later convenience. Since $\sigma_i^2 = e$ and $\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}$, any one-dimensional unitary representation $D: S_N \to U(1)$ must satisfy the conditions $D(\sigma_i)^2 = 1$ and $D(\sigma_i)D(\sigma_{i+1})D(\sigma_i) = D(\sigma_{i+1})D(\sigma_i)D(\sigma_{i+1})$, whose solutions are $D(\sigma_i) = \pm 1$ and $D(\sigma_i) = D(\sigma_{i+1})$. Hence, we have $D(\sigma_1) = \cdots = D(\sigma_{N-1}) = \pm 1$; that is, there exist two distinct maps $D^{[\pm]}$ given by

$$D^{[\pm]}(\sigma) = (\pm 1)^{\#\sigma}, \tag{24}$$

where $\#\sigma$ stands for the number of adjacent transpositions in the permutation σ . In the standard terminology, $D^{[+]}$ is the trivial representation and $D^{[-]}$ is the sign representation.⁶ Correspondingly, there exist the following two distinct timeevolution kernels for *N* identical walkers on \mathbb{Z} :

$$U_{\tau}^{[\pm]}(x, y) = \sum_{\sigma \in S_N} D^{[\pm]}(\sigma) \widetilde{U}_{\tau}(x, \sigma y)$$
$$= \sum_{\sigma \in S_N} (\pm 1)^{\#\sigma} \widetilde{U}_{\tau}(x, \sigma y).$$
(25)

Notice that Eq. (25) satisfies the identity $U_{\tau}^{[\pm]}(\sigma x, y) = (\pm 1)^{\#\sigma} U_{\tau}^{[\pm]}(x, y)$. The weight factors (24) thus describe particle-exchange phases under the permutation of identical particles. It is now obvious that the two distinct representations $D^{[\pm]}$ correspond to two distinct particle statistics: $U_{\tau}^{[+]}$ describes the time-evolution kernel for *N* identical bosons, while $U_{\tau}^{[-]}$ describes that for *N* identical fermions. For a geometrical interpretation of Eq. (25), see Fig. 2.

Example 5 (N identical walkers on a circle). Let us next consider *N* identical particles on the periodic lattice of *L* sites. In this case, the discrete group is the wreath product $\Gamma = L\mathbb{Z} \wr S_N$, whose presentation is given by

$$L\mathbb{Z} \wr S_N = \begin{pmatrix} t_1, \dots, t_N, \\ \sigma_1, \dots, \sigma_{N-1} \\ \sigma_i t_i \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}, & \sigma_i \sigma_j = \sigma_j \sigma_i \\ \sigma_i \sigma_i t_i \sigma_i = t_{i+1}, & \sigma_i t_j \sigma_i = t_j \\ \sigma_i t_i \sigma_i = t_{i+1}, & \sigma_i t_j \sigma_i = t_j \\ (j \neq i, i+1) \end{pmatrix}.$$
(26)

Here the actions of the generators t_i and σ_i are defined by Eq. (23) and

$$x_{i} := (x_1, \dots, x_{i-1}, x_i + L, x_{i+1}, \dots, x_N).$$
 (27)

Note that any element of $L\mathbb{Z} \wr S_N$ can be written as $t_1^{n_1} \dots t_N^{n_N} \sigma$, where σ is a permutation and $n_1, \dots, n_N = 0, \pm 1, \dots$. Its action on $x = (x_1, \dots, x_N)$ is given by $t_1^{n_1} \dots t_N^{n_N} \sigma x = (x_{\sigma(1)} + n_1 L, \dots, x_{\sigma(N)} + n_N L)$.

Now we have to classify one-dimensional unitary representation $D: L\mathbb{Z} \wr S_N \to U(1)$. First, the relations $\sigma_i^2 = e$ and $\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}$ imply $D(\sigma_1) = \cdots = D(\sigma_N) = \pm 1$. Second, the relation $\sigma_i t_i \sigma_i = t_{i+1}$ implies $D(\sigma_i)D(t_i)D(\sigma_i) = D(t_{i+1})$, which, together with $D(\sigma_i)^2 = 1$, leads to $D(t_1) = \cdots = D(t_N) = e^{i\theta}$, where $\theta \in \mathbb{R}/2\pi\mathbb{R}$. Thus, we have two distinct

⁶The sign representation can also be written as $D^{[-]}(\sigma) = \text{sgn}(\sigma)$, where $\text{sgn}(\sigma)$ stands for the signature of σ . It is defined by $\text{sgn}(\sigma) = \pm 1$ for even (odd) permutations.

one-parameter families of the maps $D^{[\theta,\pm]}$ given by

$$D^{[\theta,\pm]}(t_1^{n_1}\dots t_N^{n_N}\sigma) = e^{i(n_1+\dots+n_N)\theta}(\pm 1)^{\#\sigma}.$$
(28)

The time-evolution kernel for N identical walkers on $\mathbb{Z}/L\mathbb{Z}$ is therefore

$$U_{\tau}^{[\theta,\pm]}(x,y) = \sum_{n_1=-\infty}^{\infty} \cdots \sum_{n_N=-\infty}^{\infty} \sum_{\sigma \in S_N} D^{[\theta,\pm]} (t_1^{n_1} \dots t_N^{n_N} \sigma) \widetilde{U}_{\tau} (x, t_1^{n_1} \dots t_N^{n_N} \sigma y).$$
(29)

Notice that the kernel (29) satisfies the identities $U_{\tau}^{[\theta,\pm]}(\sigma x, y) = (\pm 1)^{\#\sigma} U_{\tau}^{[\theta,\pm]}(x, y)$ and $U_{\tau}^{[\theta,\pm]}(t_i x, y) = e^{i\theta} U_{\tau}^{[\theta,\pm]}(x, y)$ for any $i = 1, \ldots, N$. Physically, $U_{\tau}^{[\theta,+]}(U_{\tau}^{[\theta,-]})$ describes the system of N identical bosons (fermions) on a circle with a nonzero magnetic flux.

Example 6 (N identical walkers on the half line). Let us next consider N identical particles on the semi-infinite lattice. In this case, the discrete group is $\Gamma = \mathbb{Z}_2 \wr S_N$, where

$$\mathbb{Z}_{2} \wr S_{N} = \left\langle \begin{matrix} r_{1}, \dots, r_{N}, \\ \sigma_{1}, \dots, \sigma_{N-1} \end{matrix} \middle| \begin{matrix} r_{i}r_{j} = r_{j}r_{i}, & r_{i}^{2} = \sigma_{i}^{2} = e, \\ \sigma_{i}\sigma_{i+1}\sigma_{i} = \sigma_{i+1}\sigma_{i}\sigma_{i+1}, & \sigma_{i}\sigma_{j} = \sigma_{j}\sigma_{i} & (|i-j| \ge 2), \\ \sigma_{i}r_{i}\sigma_{i} = r_{i+1}, & \sigma_{i}r_{j}\sigma_{i} = r_{j} & (j \neq i, i+1) \end{matrix} \right\rangle.$$
(30)

The actions of the generators are defined by Eq. (23) and

$$r_i x := (x_1, \dots, x_{i-1}, 1 - x_i, x_{i+1}, \dots, x_N).$$
(31)

Note that any element of $\mathbb{Z}_2 \wr S_N$ can be written as the product $r_1^{n_1} \dots r_N^{n_N} \sigma$, where $\sigma \in S_N$ and $n_1, \dots, n_N = 0, 1$. Its action on $x = (x_1, \dots, x_N)$ is given by $r_1^{n_1} \dots r_N^{n_N} \sigma x = (\dots, x_{\sigma(i)}, \dots)$ for $n_i = 0$ and $r_1^{n_1} \dots r_N^{n_N} \sigma x = (\dots, 1 - x_{\sigma(i)}, \dots)$ for $n_i = 1$. By repeating the same procedure as above, one can show that one-dimensional unitary representation $D : \mathbb{Z}_2 \wr S_N \to U(1)$

By repeating the same procedure as above, one can show that one-dimensional unitary representation $D : \mathbb{Z}_2 \wr S_N \to U(1)$ must satisfy $D(r_1) = \cdots = D(r_N) = \pm 1$ and $D(\sigma_1) = \cdots = D(\sigma_{N-1}) = \pm 1$. Hence, there exist $2^2 = 4$ distinct maps $D^{[\phi, \pm]}$ given by

$$D^{[\phi,\pm]}(r_1^{n_1}\dots r_N^{n_N}\sigma) = e^{i(n_1+\dots+n_N)\phi}(\pm 1)^{\#\sigma},$$
(32)

where $\phi \in \{0, \pi \pmod{2\pi}\}$. The time-evolution kernel for N identical walkers on \mathbb{Z}/\mathbb{Z}_2 is therefore

$$U_{\tau}^{[\phi,\pm]}(x,y) = \sum_{n_1=0}^{1} \cdots \sum_{n_N=0}^{1} \sum_{\sigma \in S_N} D^{[\phi,\pm]} (r_1^{n_1} \dots r_N^{n_N} \sigma) \widetilde{U}_{\tau} (x, r_1^{n_1} \dots r_N^{n_N} \sigma y).$$
(33)

Notice that Eq. (33) satisfies $U_{\tau}^{[\phi,\pm]}(\sigma x, y) = (\pm 1)^{\#\sigma} U_{\tau}^{[\phi,\pm]}(x, y)$ and $U_{\tau}^{[\phi,\pm]}(r_i x, y) = e^{i\phi} U_{\tau}^{[\phi,\pm]}(x, y)$ for any i = 1, ..., N. Hence, $U_{\tau}^{[\phi,\pm]}$ describes the system of N identical bosons (fermions) that acquire the phase shift ϕ when reflected off the boundary.

Example 7 (N identical walkers on a finite interval). Let us finally consider N identical particles on a finite interval. In this case, the discrete group is $\Gamma = D_{\infty} \wr S_N$, where

$$D_{\infty} \wr S_{N} = \begin{pmatrix} t_{1}, \dots, t_{N}, \\ r_{1}, \dots, r_{N}, \\ \sigma_{1}, \dots, \sigma_{N-1} \end{pmatrix} \begin{pmatrix} t_{i}t_{j} = t_{j}t_{i}, & r_{i}r_{j} = r_{j}r_{i}, & r_{i}^{2} = \sigma_{i}^{2} = e, \\ r_{i}t_{i}r_{i} = t_{i}^{-1}, & r_{i}t_{j}r_{i} = t_{j} & (j \neq i), \\ \sigma_{i}\sigma_{i+1}\sigma_{i} = \sigma_{i+1}\sigma_{i}\sigma_{i+1}, & \sigma_{i}\sigma_{j} = \sigma_{j}\sigma_{i} & (|i-j| \ge 2), \\ \sigma_{i}r_{i}\sigma_{i} = r_{i+1}, & \sigma_{i}r_{j}\sigma_{i} = r_{j} & (j \neq i, i+1) \end{pmatrix}$$
(34)

The actions of the generators are given by Eqs. (23), (31), and

$$t_i x := (x_1, \dots, x_{i-1}, x_i + 2L, x_{i+1}, \dots, x_N).$$
(35)

We note that any element of $D_{\infty} \wr S_N$ can be written as the product $t_1^{n_1} r_1^{m_1} \dots t_N^{n_N} r_N^{m_N} \sigma$, where $\sigma \in S_N$, $n_1, \dots, n_N = 0, \pm 1, \pm 2, \dots$, and $m_1, \dots, m_N = 0, 1$. Its action is given by $t_1^{n_1} r_1^{m_1} \dots t_N^{n_N} r_N^{m_N} \sigma x = (\dots, x_{\sigma(i)} + 2n_i L, \dots)$ for $m_i = 0$ and $t_1^{n_1} r_1^{m_1} \dots t_N^{n_N} r_N^{m_N} \sigma x = (\dots, 1 - x_{\sigma(i)} + 2n_i L, \dots)$ for $m_i = 1$.

Now it is a straightforward exercise to show that there exist $2^3 = 8$ distinct one-dimensional unitary representations of the wreath product $D_{\infty} \wr S_N$. The result is the following maps:

$$D^{[\theta,\phi,\pm]}(t_1^{n_1}r_1^{m_1}\dots t_N^{n_N}r_N^{m_N}\sigma) = e^{i(n_1+\dots+n_N)\theta}e^{i(m_1+\dots+m_N)\phi}(\pm 1)^{\#\sigma},$$
(36)

where $\theta, \phi \in \{0, \pi \pmod{2\pi}\}$. Correspondingly, we have the following eight distinct time-evolution kernels for N identical walkers on \mathbb{Z}/D_{∞} :

$$U_{\tau}^{[\theta,\phi,\pm]}(x,y) = \sum_{n_1=-\infty}^{\infty} \sum_{m_1=0}^{1} \cdots \sum_{n_N=-\infty}^{\infty} \sum_{m_N=0}^{1} \sum_{\sigma \in S_N} D^{[\theta,\phi,\pm]} (t_1^{n_1} r_1^{m_1} \dots t_N^{n_N} r_N^{m_N} \sigma) \widetilde{U}_{\tau} (x, t_1^{n_1} r_1^{m_1} \dots t_N^{n_N} r_N^{m_N} \sigma y).$$
(37)

Physically, $U_{\tau}^{[\theta,\phi,\pm]}$ describes the system of N identical bosons (fermions) that acquire the phase shifts ϕ and $\theta + \phi$ when reflected off the boundaries x = 1 and x = L, respectively.

IV. ASIDES

Now, there exist several other quantities that can be constructed in exactly the same way as for the time-evolution kernel (4). Examples include the resolvent kernel (Green's function) and the canonical density matrix (density matrix in the canonical ensemble). Another example is a unitary representation of an arbitrary group *G* on a (tensor-product) Hilbert space, which includes the time-evolution kernel in discrete-time quantum walk. In this section, we shall briefly discuss the construction of these quantities on the orbit space Λ/Γ .

A. Resolvent kernel

Let us first start with the resolvent kernel—a matrix element of the resolvent operator in position space. Let H be the Hamiltonian operator of the system. Then, the resolvent operator $G_E = (EI - H)^{-1}$ for ImE > 0 and the time-evolution operator $U_{\tau} = e^{-iH\tau}$ for $\tau > 0$ are transformed into one another through the Laplace transform $i(EI - H)^{-1} = \int_0^\infty d\tau e^{-iH\tau} e^{iE\tau}$ and the inverse Laplace transform $e^{-iH\tau} = \int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{dE}{2\pi} i(EI - H)^{-1} e^{-iE\tau}$, respectively, where ϵ is an arbitrary positive real. Consequently, the matrix elements $U_{\tau}(x, y) = \langle x | U_{\tau} | y \rangle$ and $G_E(x, y) = \langle x | G_E | y \rangle$ are mutually related through the following:

$$iG_E(x, y) = \int_0^\infty d\tau \ U_\tau(x, y) e^{iE\tau} \quad \text{for} \quad \text{Im}E > 0, \quad (38a)$$
$$U_\tau(x, y) = \int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{dE}{2\pi} \ iG_E(x, y) e^{-iE\tau} \quad \text{for} \quad \tau > 0.$$
(38b)

Hence, by applying the Laplace transform to formula (4), we find that the resolvent kernel on Λ/Γ takes the following form:

$$G_E(x, y) = \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{G}_E(x, \gamma y), \qquad (39)$$

where $i\widetilde{G}_E(x, y) = \int_0^\infty d\tau \ \widetilde{U}_\tau(x, y) e^{iE\tau}$ (ImE > 0) is the resolvent kernel on Λ .

An immediate application of the above formula is the local density of states given by $\rho_E(x) = \langle x | \delta(EI - H) | x \rangle$. In fact, by using the identity

$$\lim_{I \to 0^+} (EI - H)^{-1} = \mathscr{P}(EI - H)^{-1} - i\pi \delta(EI - H),$$
(40)

where \mathscr{P} stands for the Cauchy principal value, we find $\text{Im}G_E(x, x) = \text{Im}\langle x | (EI - H)^{-1} | x \rangle = -\pi \langle x | \delta(EI - H)$

 $|x\rangle = -\pi \rho_E(x)$ in the limit Im $E \to 0_+$. Thus,

$$\rho_E(x) = -\frac{1}{\pi} \operatorname{Im} \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{G}_E(x, \gamma x) \quad \text{as} \quad \operatorname{Im} E \to 0_+.$$
(41)

The density of states $\rho_E = \text{tr}\delta(EI - H)$ then takes the form $\rho_E = -(1/\pi)\text{Im}\sum_{x \in \Lambda/\Gamma}\sum_{\gamma \in \Gamma} D(\gamma)\widetilde{G}_E(x, \gamma x).$

B. Canonical density matrix

Let us next consider the canonical density matrix on Λ/Γ . In thermal equilibrium at temperature β^{-1} , the canonical density matrix is given by $\rho_{\beta} = U_{-i\beta}/Z(\beta)$, where $U_{-i\beta} = e^{-\beta H}$ is the Gibbs operator and $Z(\beta) = \text{tr}U_{-i\beta}$ is the canonical partition function. Note that the Gibbs operator satisfies the composition law $U_{-i\beta_1}U_{-i\beta_2} = U_{-i(\beta_1+\beta_2)}$, the hermiticity $U_{-i\beta}^{\dagger} = U_{-i\beta}$, and the initial condition $U_0 = I$. Its matrix elements (heat kernel) $U_{-i\beta}(x, y) = \langle x | e^{-\beta H} | y \rangle$ must then satisfy these conditions as well. Namely, we must have $\sum_{z \in \Lambda/\Gamma} U_{-i\beta_1}(x, z)U_{-i\beta_2}(z, y) = U_{-i(\beta_1+\beta_2)}(x, y)$, $\overline{U_{-i\beta}(x, y)} = U_{-i\beta}(y, x)$, and $U_0(x, y) = \delta_{x,y}$. Under these conditions, one can again show that $U_{-i\beta}(x, y)$ can be written as $U_{-i\beta}(x, y) = \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{-i\beta}(x, \gamma y)$. Hence the matrix elements of the canonical density matrix are

$$\rho_{\beta}(x, y) = \frac{1}{Z(\beta)} \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{-i\beta}(x, \gamma y), \qquad (42)$$

where $\rho_{\beta}(x, y) = \langle x | \rho_{\beta} | y \rangle$. Here $Z(\beta)$ is the canonical partition function given by

$$Z(\beta) = \sum_{x \in \Lambda/\Gamma} \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_{-i\beta}(x, \gamma x).$$
(43)

We note that the partition function (43) can also be written as $Z(\beta) = \sum_{x \in \Lambda/\Gamma} \sum_{\gamma \in \Gamma} D(\gamma) \langle x | e^{-\beta \widetilde{H}} | \gamma x \rangle =$ $\sum_{\gamma \in \Gamma} D(\gamma) \operatorname{tr}(e^{-\beta \widetilde{H}} W_{\gamma})$, where \widetilde{H} is the Hamiltonian operator on Λ and W_{γ} is a unitary operator defined by $W_{\gamma} | x \rangle = | \gamma x \rangle$.

C. Unitary representations of arbitrary groups on a tensor-product Hilbert space

As mentioned in the beginning of Sec. II, our main formula (4) is also applicable to discrete-time quantum walk, where the time τ takes discrete values and the one-particle Hilbert space is the tensor product of the position and coin Hilbert spaces. In this section, we shall see this from a more general perspective: the construction of matrix elements of a unitary representation of an arbitrary group *G* on a tensor-product Hilbert space. The time-evolution kernel in discrete-time

quantum walk just corresponds to the special case $G = \mathbb{Z}$ (the additive group of integers).

To begin with, let $\{U_g \in U(\mathcal{H}) : g \in G\}$ be a unitary representation of G on the tensor-product Hilbert space $\mathcal{H} = \mathcal{H}_{\text{position}} \otimes \mathcal{H}_{\text{coin}}$, where $U(\mathcal{H})$ stands for the set of unitary operators on \mathcal{H} , $\mathcal{H}_{\text{position}} = l^2(\Lambda/\Gamma)$ is the set of square-summable sequences on the orbit space Λ/Γ , and $\mathcal{H}_{\text{coin}} = \mathbb{C}^d$ is the *d*-dimensional complex vector space that describes internal degrees of freedom of particles. Let $\{|x\rangle\}$ and $\{|i\rangle\}$ be complete orthonormal systems of $\mathcal{H}_{\text{position}}$ and $\mathcal{H}_{\text{coin}}$, respectively. The set $\{|x\rangle \otimes |i\rangle\}$ then provides a complete orthonormal system of the total Hilbert space \mathcal{H} such that the matrix elements of U_g can be defined as $U_g(x, i; y, j) = (\langle x | \otimes \langle i |)U_g(|y \otimes | j \rangle)$.

We now define $U_g(x, y)$ as the following $d \times d$ matrix:

$$U_{g}(x, y) := \begin{pmatrix} U_{g}(x, 1; y, 1) & \cdots & U_{g}(x, 1; y, d) \\ \vdots & \ddots & \vdots \\ U_{g}(x, d; y, 1) & \cdots & U_{g}(x, d; y, d) \end{pmatrix}.$$
 (44)

Since the unitary representation must satisfy the group composition law $U_{g_1}U_{g_2} = U_{g_1g_2}$, the unitarity $U_g^{\dagger}(=U_g^{-1}) = U_{g^{-1}}$, and the initial condition $U_e = I$, matrix (44) must also satisfy the following properties:

$$\sum_{z \in \Lambda/\Gamma} U_{g_1}(x, z) U_{g_2}(z, y) = U_{g_1g_2}(x, y),$$
(45a)

$$\overline{{}^{t}U_{g}(x,y)} = U_{g^{-1}}(y,x),$$
 (45b)

$$U_e(x, y) = \delta_{x, y} \mathbf{1}, \tag{45c}$$

where $x, y \in \Lambda/\Gamma$. Here *t* and **1** stand for the matrix transpose and the $d \times d$ identity matrix, respectively. Now it is a straightforward exercise to show that matrix (44) can be written as

$$U_g(x, y) = \sum_{\gamma \in \Gamma} D(\gamma) \widetilde{U}_g(x, \gamma y), \tag{46}$$

where $\widetilde{U}_g(x, y)$ is a $d \times d$ matrix subject to the conditions $\sum_{z \in \Lambda} \widetilde{U}_{g_1}(x, z) \widetilde{U}_{g_2}(z, y) = \widetilde{U}_{g_1g_2}(x, y), \quad \overline{U}_g(x, y) = \widetilde{U}_{g^{-1}}(y, x),$ $\widetilde{U}_e(x, y) = \delta_{x,y} \mathbf{1}, \text{ and } \widetilde{U}_g(\gamma x, \gamma y) = \widetilde{U}_g(x, y) \text{ for any } x, y \in \Lambda$ and $\gamma \in \Gamma$. It is also straightforward to show that Eq. (46) satisfies the following boundary condition:

$$U_g(\gamma x, y) = D(\gamma)U_g(x, y), \quad \forall \gamma \in \Gamma.$$
(47)

It is now obvious that Eq. (46) provides the time-evolution kernel of continuous-time quantum walk with internal degrees of freedom when $G = \mathbb{R}$ (the additive group of real numbers) and of discrete-time quantum walk when $G = \mathbb{Z}$ (the additive group of integers). It is also obvious that the examples presented in Sec. III apply to discrete-time quantum walk as well.

V. CONCLUSION

Inspired by the covering-space method in path integral on multiply connected spaces, we have developed a general theory of quantum walk on orbit spaces. In this note, we have proved the universal formulas for time-evolution kernels, resolvent kernels, canonical density matrices, and unitary representations of arbitrary groups in continuous- and discrete-time quantum walks on the orbit space Λ/Γ , where Λ is an arbitrary lattice and Γ is a discrete group whose action on Λ has no fixed points. All of these quantities are given by summations over the orbit of initial point on Λ , where each orbit is weighted by a phase factor given by a one-dimensional unitary representation of Λ .

There are several advantages of this orbit-space method. A main advantage is its universality: our formulas are just based on geometric and group-theoretic structures of configuration spaces so that they are robust against any perturbations or interparticle interactions as long as boundary conditions (8) remain unchanged. Another advantage is its computational simplicity: in our formalism, one just needs to compute matrix elements on Λ , which is generally much easier than computations on Λ/Γ .

Finally, let us comment on one possible future direction of this work. A promising direction would be a generalization of our formulas to the problem of identical walkers on graphs. Recent studies have shown that exotic statistics may show up in many-body problems of identical particles on graphs [31–35]. Such exotic statistics are generalizations of braid-group statistics in two dimensions. Hence, just as in topological quantum computation using anyons [36], they would have potential applications in quantum computer science. Our formalism and its generalization may well serve as a basic tool for studying the dynamics as well as thermodynamics of such systems.

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APPENDIX: SAMPLE COMPUTATIONS

Continuous-time quantum walk is just equivalent to tightbinding models in condensed matter physics. The advantage of this perspective is that it is straightforward to study many-particle problems by using the second-quantization formalism. In this section, we study tight-binding models for free spinless particles in one dimension and present sample computations that justify the formulas in Sec. III.

1. Tight-binding model on the infinite line

Let us first consider spinless particles on the integer lattice \mathbb{Z} only with a nearest-neighbor coupling. In the secondquantization formalism, the Hamiltonian operator is given by

$$\widetilde{H} = -\frac{\omega}{2} \sum_{x \in \mathbb{Z}} (a_{x+1}^{\dagger} a_x + a_x^{\dagger} a_{x+1}), \qquad (A1)$$

where $\omega(>0)$ is a hopping parameter. a_x and a_x^{\dagger} are annihilation and creation operators for spinless bosons (fermions) and subject to the following (anti)commutation relations:

$$[a_x, a_y^{\dagger}]_{\mp} = \delta_{x,y}$$
 and $[a_x, a_y]_{\mp} = 0,$ (A2)

where $[A, B]_{\mp} = AB \mp BA$.

Let $|0\rangle$ be the Fock vacuum that satisfies $a_x|0\rangle = 0$ for all *x*. The time-evolution kernel in the one-particle sector of the

model is then given by

$$\widetilde{U}_{\tau}(x, y) = \langle x | e^{-i\widetilde{H}\tau} | y \rangle, \tag{A3}$$

where $|x\rangle = a_x^{\dagger}|0\rangle$ is the position-space basis in the oneparticle sector. It satisfies the orthonormality $\langle x|y\rangle = \langle 0|a_x a_y^{\dagger}|0\rangle = \delta_{x,y}$ for both bosons and fermions. In order to calculate the matrix element (A3), we first diagonalize the Hamiltonian operator, which can be achieved by the following Fourier integral:

$$a_x = \int_{-\pi}^{\pi} \frac{dp}{2\pi} \,\widetilde{a}_p \mathrm{e}^{ipx},\tag{A4}$$

where \tilde{a}_p and \tilde{a}_p^{\dagger} satisfy $[\tilde{a}_p, \tilde{a}_q^{\dagger}]_{\mp} = 2\pi\delta(p-q)$ and $[\tilde{a}_p, \tilde{a}_q]_{\mp} = 0$ for any $p, q \in (-\pi, \pi)$. By substituting Eq. (A4) into Eq. (A3), we obtain

$$\widetilde{H} = \int_{-\pi}^{\pi} \frac{dp}{2\pi} \varepsilon_p \widetilde{a}_p^{\dagger} \widetilde{a}_p, \qquad (A5)$$

where $\varepsilon_p = -\omega \cos(p)$ is the single-particle energy eigenvalue. It is now easy to see that the time-evolution kernel (A3) takes the following form:

$$\begin{split} \tilde{U}_{\tau}(x,y) &= \langle 0|a_{x}e^{-iH\tau}a_{y}^{\dagger}|0\rangle \\ &= \int_{-\pi}^{\pi} \frac{dp}{2\pi} \int_{-\pi}^{\pi} \frac{dq}{2\pi} \langle 0|\tilde{a}_{p}e^{-i\tilde{H}\tau}\tilde{a}_{q}^{\dagger}|0\rangle e^{ipx-iqy} \\ &= \int_{-\pi}^{\pi} \frac{dp}{2\pi} \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-i\varepsilon_{q}t} \langle 0|\tilde{a}_{p}\tilde{a}_{q}^{\dagger}|0\rangle e^{ipx-iqy} \\ &= \int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{i\omega\tau\cos(p)} e^{ip(x-y)}, \end{split}$$
(A6)

where in the third equality we have used $e^{-iH\tau}\tilde{a}_{q}^{\dagger}|0\rangle = e^{-i\epsilon_{q}t}\tilde{a}_{q}^{\dagger}|0\rangle$, which follows from $e^{-iH\tau}\tilde{a}_{q}^{\dagger}e^{iH\tau} = e^{-i\epsilon_{q}t}\tilde{a}_{q}^{\dagger}$ and $e^{-iH\tau}|0\rangle = |0\rangle$ (or, equivalently, $[H, \tilde{a}_{q}^{\dagger}] = \epsilon_{q}\tilde{a}_{q}^{\dagger}$ and $H|0\rangle = 0$). The fourth equality follows from $\langle 0|\tilde{a}_{p}\tilde{a}_{q}^{\dagger}|0\rangle = 2\pi\delta(p-q)$ for both bosons and fermions. To evaluate the last integral in Eq. (A6), we note that $e^{i\omega\tau\cos(p)}$ is a generating function of the Bessel function of the first kind J_{n} . In fact,

$$e^{i\omega\tau\cos(p)} = \sum_{n=-\infty}^{\infty} e^{in\left(p+\frac{\pi}{2}\right)} J_n(\omega\tau)$$
$$= \sum_{n=-\infty}^{\infty} e^{i\frac{\pi}{2}|n|} J_{|n|}(\omega\tau) e^{-inp}, \qquad (A7)$$

where the second equality follows from $J_{-n}(x) = e^{in\pi} J_n(x)$. By substituting Eq. (A7) into Eq. (A6) and then using the orthogonal relation $\int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{ip(x-y-n)} = \delta_{n,x-y}$, we obtain

$$\widetilde{U}_{\tau}(x,y) = e^{i\frac{\pi}{2}|x-y|} J_{|x-y|}(\omega\tau), \quad \forall x, y \in \mathbb{Z}.$$
 (A8)

This is the well-known transition amplitude for a single walker on the lattice \mathbb{Z} (see, e.g., Ref. [37]). Note that Eq. (A8) satisfies the composition law (3a), the unitarity (3b), and the initial condition (3c), which follow from the addition theorem $J_{n_1-n_2}(x_1 + x_2)e^{i\frac{\pi}{2}(n_1-n_2)} = \sum_{n \in \mathbb{Z}} J_{n_1-n}(x_1)J_{n_2-n}(x_2)e^{i\frac{\pi}{2}(n_1-n)}e^{i\frac{\pi}{2}(n_2-n)}$ $(n_1, n_2 \in \mathbb{Z})$, the analytic continuation $J_n(e^{i\pi}x) = e^{in\pi}J_n(x)$, and $J_n(0) = \delta_{n,0}$, respectively. Note also that Eq. (A8) enjoys the translation

invariance $\widetilde{U}_{\tau}(x+z, y+z) = \widetilde{U}_{\tau}(x, y)$ and the reflection invariance $\widetilde{U}_{\tau}(z-x, z-y) = \widetilde{U}_{\tau}(x, y)$ for any $x, y, z \in \mathbb{Z}$. As we shall see shortly, Eq. (A8) provides the building block for the construction of time-evolution kernels for a free particle on a circle, the half line, and a finite interval.

Several comments are in order.

(1) Resolvent kernel for a single walker: As discussed in Sec. IV A, the resolvent kernel (Green's function) is given by the Laplace transform of $\widetilde{U}_{\tau}(x, y)$. Let *E* be a complex number with ImE > 0. Then we have

$$i\widetilde{G}_{E}(x, y) = \int_{0}^{\infty} d\tau \, \widetilde{U}_{\tau}(x, y) e^{iE\tau}$$
$$= \int_{-\pi}^{\pi} \frac{dp}{2\pi} \, \frac{ie^{ip(x-y)}}{E + \omega \cos(p)}$$
$$= \frac{2i}{\omega} \oint_{|z|=1} \frac{dz}{2\pi i} \, \frac{z^{|x-y|}}{z^{2} + \frac{2E}{\omega}z + 1}, \qquad (A9)$$

where in the second equality we have substituted the last line of Eq. (A6) and performed the integration with respect to τ . In the last equality we have changed the integration variable from *p* to $z = e^{ip}$, where the integration is over the closed loop |z| = 1 in the counterclockwise direction. By using the residue theorem we find

$$i\widetilde{G}_E(x,y) = \frac{e^{ip|x-y|}}{\omega\sin(p)},$$
(A10)

where we have parametrized the energy as $E = -\omega \cos(p)$ with $\operatorname{Re} p \in (0, \pi)$ and $\operatorname{Im} p \in (0, \infty)$. Equation (A10) provides the building block for the construction of single-particle resolvent kernels on a circle, the half line, and a finite interval.

(2) *Heat kernel for a single walker.* The matrix element of the Gibbs operator $e^{-\beta \tilde{H}}$ can be calculated in exactly the same way as for $\tilde{U}_{\tau}(x, y)$. Under the substitution $\tau \to -i\beta$ in Eq. (A6) we find

$$\widetilde{U}_{-i\beta}(x, y) = \int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{\beta \omega \cos(p)} e^{ip(x-y)}$$
$$= I_{x-y}(\beta \omega), \qquad (A11)$$

where $I_n(x) = I_{-n}(x)$ stands for the modified Bessel function of the first kind. Here in the last line we have used the fact that $e^{\beta \omega \cos(p)}$ is the generating function of $I_n(\beta \omega)$. In fact,

$$e^{\beta\omega\cos(p)} = \sum_{n=-\infty}^{\infty} I_n(\beta\omega) e^{-inp}.$$
 (A12)

By substituting this into the first line and using the orthogonal relation $\int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{ip(x-y-n)} = \delta_{n,x-y}$, we arrive at Eq. (A11). As discussed in Sec. IV B, Eq. (A11) provides the building block for the construction of canonical density matrices for free particles on a circle and a finite interval.

(3) *Time-evolution kernel for N identical walkers*. In the second-quantization formalism, it is easy to generalize the above results to many-particle problems. First, the position-space basis in the N-particle sector is given by

$$|x_1,\ldots,x_N\rangle := a_{x_1}^{\dagger}\ldots a_{x_N}^{\dagger}|0\rangle. \tag{A13}$$

Notice that Eq. (A13) satisfies the orthonormality condition on the orbit space $(\mathbb{Z}^N - \Delta_N)/S_N \cong \{(x_1, \dots, x_N) \in \mathbb{Z}^N :$ $x_1 < \cdots < x_N$. In fact, for $x_1 < \cdots < x_N$ and $y_1 < \cdots < y_N$, we have

$$\langle x_1, \dots, x_N | y_1, \dots, y_N \rangle = \langle 0 | a_{x_N} \dots a_{x_1} a_{y_1}^{\dagger} \dots a_{y_N}^{\dagger} | 0 \rangle$$

$$= \sum_{\sigma \in S_N} (\pm 1)^{\#\sigma} \delta_{x_{\sigma(1)}, y_1} \dots \delta_{x_{\sigma(N)}, y_N}$$

$$= \delta_{x_1, y_1} \dots \delta_{x_N, y_N},$$
(A14)

where the last line follows from the fact that $(x_{\sigma(1)}, \ldots, x_{\sigma(N)})$ and (y_1, \ldots, y_N) cannot be equal except for $\sigma = e$. It is now easy to show that the time-evolution kernels for N identical bosons and fermions take the following forms:⁷

$$\begin{aligned} \langle x_1, \dots, x_N | e^{-iH\tau} | y_1, \dots, y_N \rangle \\ &= \langle 0 | a_{x_N} \dots a_{x_1} e^{-i\widetilde{H}\tau} a_{y_1}^{\dagger} \dots a_{y_N}^{\dagger} | 0 \rangle \\ &= \left[\prod_{j=1}^N \int_{-\pi}^{\pi} \frac{dp_j}{2\pi} \int_{-\pi}^{\pi} \frac{dq_j}{2\pi} \right] e^{i\omega\tau(\cos(q_1) + \dots + \cos(q_N))} \\ &\times \langle 0 | \widetilde{a}_{p_N} \dots \widetilde{a}_{p_1} \widetilde{a}_{q_1}^{\dagger} \dots \widetilde{a}_{q_N}^{\dagger} | 0 \rangle e^{ip_1x_1 + \dots + ip_Nx_N - iq_1y_1 - \dots - iq_Ny_N} \\ &= \sum_{j=1}^N (\pm 1)^{\#\sigma} \prod_{j=1}^N e^{i\frac{\pi}{2} | x_j - y_\sigma(j) | J_{\sigma_j}} e^{i(x_j)} e^{i(x_$$

$$= \sum_{\sigma \in S_N} (\pm 1)^{\#\sigma} \prod_{j=1} e^{i \frac{\pi}{2} |x_j - y_{\sigma(j)}|} J_{|x_j - y_{\sigma(j)}|}(\omega \tau).$$
(A15)

This equation can be used to construct the time-evolution kernels for free identical walkers on a circle, the half line, and a finite interval.

2. Tight-binding model on a circle

Let us next consider the tight-binding model for free spinless particles on the periodic lattice $\{1, 2, ..., L \pmod{L}\}$ subject to the twisted boundary condition $a_{x+L} = e^{i\theta}a_x$. As we shall see shortly, the following Hamiltonian operator yields the desired results:

$$H = -\frac{\omega}{2} \sum_{x=1}^{L} (a_{x+1}^{\dagger} a_x + a_x^{\dagger} a_{x+1}), \text{ where } a_{L+1} \equiv e^{i\theta} a_1.$$
(A16)

In the following, we assume that θ ranges from 0 to 2π .

In order to compute the time-evolution kernel, we first have to diagonalize the Hamiltonian operator (A16), which can be done by using the mode expansion. Under the twisted boundary condition, the annihilation operator can be expanded into the following:

$$a_x = \frac{1}{\sqrt{L}} \sum_{p=0}^{L-1} \widetilde{a}_p e^{i\frac{2p\pi+\theta}{L}x},$$
(A17)

where \tilde{a}_p and \tilde{a}_p^{\dagger} satisfy $[\tilde{a}_p, \tilde{a}_q^{\dagger}]_{\mp} = \delta_{p,q}$ and $[\tilde{a}_p, \tilde{a}_q]_{\mp} = 0$ for any $p, q \in \{0, 1, \dots, L-1\}$. By substituting Eq. (A17) into Eq. (A16), we find that the Hamiltonian operator is diagonalized as follows:

$$H = \sum_{p=0}^{L-1} \varepsilon_p \widetilde{a}_p^{\dagger} \widetilde{a}_p, \qquad (A18)$$

where $\varepsilon_p = -\omega \cos(\frac{2p\pi + \theta}{L})$ is the single-particle energy eigenvalue on the periodic lattice.

Now it is easy to compute the time-evolution kernel in the one-particle sector. A straightforward calculation gives

$$\begin{aligned} U_{\tau}^{[\theta]}(x, y) &= \langle x| \mathrm{e}^{-iH\tau} |y\rangle \\ &= \langle 0|a_{x} \mathrm{e}^{-iH\tau} a_{y}^{\dagger}|0\rangle \\ &= \frac{1}{L} \sum_{p=0}^{L-1} \sum_{q=0}^{L-1} \langle 0|\widetilde{a}_{p} \mathrm{e}^{-iH\tau} \widetilde{a}_{q}^{\dagger}|0\rangle \mathrm{e}^{i\frac{2p\pi+\theta}{L}x-i\frac{2q\pi+\theta}{L}y} \\ &= \frac{1}{L} \sum_{p=0}^{L-1} \sum_{q=0}^{L-1} \mathrm{e}^{-i\varepsilon_{q}\tau} \langle 0|\widetilde{a}_{p} \widetilde{a}_{q}^{\dagger}|0\rangle \mathrm{e}^{i\frac{2p\pi+\theta}{L}x-i\frac{2q\pi+\theta}{L}y} \\ &= \frac{1}{L} \sum_{p=0}^{L-1} \mathrm{e}^{i\omega\tau} \cos(\frac{2p\pi+\theta}{L}) \mathrm{e}^{i\frac{2p\pi+\theta}{L}(x-y)}, \end{aligned}$$
(A19)

where we have used $e^{-iH\tau} \tilde{a}_{q}^{\dagger}|0\rangle = e^{-i\varepsilon_{q}\tau} \tilde{a}_{q}^{\dagger}|0\rangle$ in the fourth line and $\langle 0|\tilde{a}_{p}\tilde{a}_{q}^{\dagger}|0\rangle = \delta_{p,q}$ in the last line. Notice that Eq. (A19) is the summation over the energy spectrum. In order to obtain the summation over winding numbers, we therefore have to perform a resummation, which can be done by using Eq. (A7). By substituting $e^{i\omega t \cos(\frac{2p\pi+\theta}{L})} = \sum_{m \in \mathbb{Z}} e^{i\frac{\pi}{2}|m|} J_{|m|}(\omega t) e^{-im\frac{2p\pi+\theta}{L}}$ into Eq. (A19) and using the orthogonal relation $(1/L) \sum_{p=0}^{L-1} e^{i\frac{2p\pi+\theta}{L}(x-y-m)} = e^{in\theta} \delta_{m,x-y-nL}$ $(n \in \mathbb{Z})$, we find that the time-evolution kernel (A19) can be put into the following alternative equivalent form:⁸

$$U_{\tau}^{\left[\theta\right]}(x,y) = \sum_{n=-\infty}^{\infty} e^{in\theta} e^{i\frac{\pi}{2}|x-y-nL|} J_{|x-y-nL|}(\omega\tau), \quad (A20)$$

which exactly coincides with Eq. (15) with $\tilde{U}_{\tau}(\cdot, \cdot)$ given by Eq. (A8). This sample computation implies that there is an equivalence (or duality) between the summation over energy spectrum and the summation over a particle's trajectories, which is the heart of the trace formula in harmonic analysis and representation theory (see, e.g., Ref. [39]). In this respect, one could say that our formula is a version of the trace formula in lattice geometry.

Although we omit the details, it is not difficult to show that the resolvent kernel, the canonical density matrix, and the time-evolution kernel for N identical particles all coincide with the universal formulas.

We note in closing that the parameter θ can be removed from the twisted boundary condition under the gauge transformation $a_x \mapsto V_{\theta} a_x V_{\theta}^{-1} = e^{i\frac{\theta}{L}x} a_x$, where V_{θ} is a unitary operator given by $V_{\theta} = \exp(-i\frac{\theta}{L}\sum_{x=1}^{L}xa_x^{\dagger}a_x)$ (see, e.g., Ref. [40]). In fact, a straightforward calculation

⁷It should be noted that $\widetilde{U}_{\tau}(x_1, \ldots, x_N, y_1, \ldots, y_N) = \prod_{j=1}^{N} e^{i\frac{\pi}{2}|x_j-y_j|} J_{|x_j-y_j|}(\omega\tau)$ is equivalent to a single-particle time-evolution kernel on \mathbb{Z}^N rather than $\mathbb{Z}^N - \Delta_N$. As noted in the beginning of Sec. III B, in this note we will not touch upon this type of issue related to the fixed points of S_N .

⁸The case $\theta = 0$ was noted in Ref. [38].

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$$V_{\theta}HV_{\theta}^{-1} = -\frac{\omega}{2}\sum_{x=1}^{L} (e^{-i\theta/L}a_{x+1}^{\dagger}a_{x} + e^{+i\theta/L}a_{x}^{\dagger}a_{x+1}),$$

here $a_{L+1} \equiv a_{1}.$ (A21)

The time-evolution kernel in the one-particle sector for this Hamiltonian coincides with Eq. (A20) up to a phase factor $e^{i\frac{\theta}{L}(x-y)}$ and hence is physically equivalent.

3. Tight-binding model on the half line

Let us next consider the tight-binding model on the semiinfinite lattice $\{1, 2, ...\}$ with the boundary condition $a_0 = e^{i\phi}a_1$, where $\phi \in \{0, \pi\}$. The Hamiltonian operator that ensures this boundary condition is given by

$$H = -\frac{\omega}{2} \sum_{x=1}^{\infty} (a_{x+1}^{\dagger} a_x + a_x^{\dagger} a_{x+1}) - \frac{\omega}{2} e^{i\phi} a_1^{\dagger} a_1.$$
 (A22)

By substituting the mode expansion

$$a_{x} = \int_{0}^{\pi} \frac{dp}{2\pi} \,\widetilde{a}_{p} (\mathrm{e}^{-ipx} + \mathrm{e}^{i\phi} \mathrm{e}^{-ip(1-x)}), \tag{A23}$$

we get the following diagonalized Hamiltonian operator:

$$H = \int_0^\pi \frac{dp}{2\pi} \,\varepsilon_p \widetilde{a}_p^\dagger \widetilde{a}_p, \qquad (A24)$$

where $\varepsilon_p = -\omega \cos(p)$ is the single-particle energy eigenvalue. The time-evolution kernel for a single walker is

given by

$$\begin{aligned} U_{\tau}^{[\phi]}(x, y) \\ &= \langle 0 | a_{x} e^{-iH\tau} a_{y}^{\dagger} | 0 \rangle \\ &= \int_{0}^{\pi} \frac{dp}{2\pi} e^{-i\varepsilon_{p}\tau} (e^{-ipx} + e^{i\phi} e^{-ip(1-x)}) (e^{ipy} + e^{i\phi} e^{ip(1-y)}) \\ &= \int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{i\omega\tau \cos(p)} (e^{ip(x-y)} + e^{i\phi} e^{ip(x-1+y)}) \\ &= e^{i\frac{\pi}{2}|x-y|} J_{|x-y|}(\omega\tau) + e^{i\phi} e^{i\frac{\pi}{2}|x-1+y|} J_{|x-1+y|}(\omega\tau), \end{aligned}$$
(A25)

which exactly coincides with Eq. (18). Other quantities can be calculated in a similar way and coincide with the universal formulas.

We note that the model that satisfies the Dirichlet boundary condition $a_x = 0$ at x = 0 is described by the Hamiltonian operator $H = -(\omega/2) \sum_{x=1}^{\infty} (a_{x+1}^{\dagger}a_x + a_x^{\dagger}a_{x+1})$. In this case, the time-evolution kernel coincides with another formula discussed in example 2 in Sec. III A.

4. Tight-binding model on a finite interval

Let us finally quickly study the tight-binding model on the finite lattice $\{1, 2, ..., L\}$ with the boundary conditions $a_0 = e^{i\phi}a_1$ and $a_{L+1} = e^{i(\theta+\phi)}a_L$, where $\theta, \phi \in \{0, \pi\}$. The Hamiltonian operator is given by

$$H = -\frac{\omega}{2} \sum_{x=1}^{L-1} (a_{x+1}^{\dagger} a_x + a_x^{\dagger} a_{x+1}) - \frac{\omega}{2} e^{i\phi} a_1^{\dagger} a_1 - \frac{\omega}{2} e^{i(\theta+\phi)} a_L^{\dagger} a_L.$$
(A26)

This operator can be diagonalized by using the following mode expansions:

$$a_{x} = \begin{cases} \frac{1}{\sqrt{L}} \widetilde{a}_{0} + \frac{1}{\sqrt{2L}} \sum_{p=1}^{L-1} \widetilde{a}_{p} \left(e^{-i\frac{2p\pi}{2L}x} + e^{-i\frac{2p\pi}{2L}(1-x)} \right) & \text{for } \theta = 0 \& \phi = 0; \\ \frac{1}{\sqrt{2L}} \sum_{p=1}^{L-1} \widetilde{a}_{p} \left(e^{-i\frac{2p\pi}{2L}x} - e^{-i\frac{2p\pi}{2L}(1-x)} \right) + \frac{1}{\sqrt{L}} \widetilde{a}_{L}(-1)^{x} & \text{for } \theta = 0 \& \phi = \pi; \\ \frac{1}{\sqrt{2L}} \sum_{p=0}^{L-1} \widetilde{a}_{p} \left(e^{-i\frac{2p\pi}{2L}x} + e^{i\phi} e^{-i\frac{2p\pi}{2L}(1-x)} \right) & \text{otherwise.} \end{cases}$$
(A27)

In fact, by substituting these into Eq. (A26) we find

$$H = \begin{cases} \sum_{p=1}^{L} \varepsilon_p \widetilde{a}_p^{\dagger} \widetilde{a}_p & \text{for } \theta = 0 \& \phi = \pi; \\ \sum_{p=0}^{L-1} \varepsilon_p \widetilde{a}_p^{\dagger} \widetilde{a}_p & \text{otherwise,} \end{cases}$$
(A28)

where $\varepsilon_p = -\omega \cos(\frac{2p\pi + \theta}{2L})$ for any $\theta, \phi \in \{0, \pi\}$. It is not difficult to show that the time-evolution kernel for a single walker can be put into the following expression irrespective of the values of θ and ϕ :

$$U_{\tau}^{[\theta,\phi]}(x,y) = \langle 0|a_{x}e^{-iH\tau}a_{y}^{\dagger}|0\rangle = \frac{1}{2L}\sum_{p=0}^{2L-1} e^{i\omega\tau\cos\left(\frac{2p\pi+\theta}{2L}\right)} \left(e^{i\frac{2p\pi+\theta}{2L}(x-y)} + e^{i\phi}e^{i\frac{2p\pi+\theta}{2L}(x-1+y)}\right).$$
(A29)

Note that this is the summation over the energy spectrum. However, as was done in Appendix A2, this summation can be rewritten into the following summation over the bouncing numbers off the boundaries:

$$U_{\tau}^{[\theta,\phi]}(x,y) = \sum_{n=-\infty}^{\infty} \left[e^{in\theta} e^{i\frac{\pi}{2}|x-y-2nL|} J_{|x-y-2nL|}(\omega\tau) + e^{in\theta} e^{i\phi} e^{i\frac{\pi}{2}|x-1+y-2nL|} J_{|x-1+y-2nL|}(\omega\tau) \right],$$
(A30)

which exactly coincides with the universal formula (21).

If one wants to study the model that satisfies the Dirichlet boundary conditions $a_x = 0$ at x = 0 and x = L + 1, one should use $H = -(\omega/2) \sum_{x=1}^{L-1} (a_{x+1}^{\dagger} a_x + a_x^{\dagger} a_{x+1})$. In this case, the time-evolution kernel coincides with another formula discussed in example 3 in Sec. III A.

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