Effective dynamics from minimizing dissipation

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It is known that the same physical system can be described by different effective theories depending on the scale at which it is observed. In this work, we formulate a prescription for finding the unitary that best approximates the large-scale dynamics of a quantum system evolving discretely in time, as it is the case for digital quantum simulators. We consider the situation in which the degrees of freedom of the system can be divided between an IR part that we can observe and a UV part that we cannot observe. Following a principle of minimal dissipation, our goal is to find the unitary dynamics that best approximates the (generally nonunitary) time evolution of the IR degrees of freedom. We first prove that when the IR and UV degrees of freedom are weakly coupled, the unitary that maximizes the fidelity is given by a mean-field dynamics and the error is given by a sum of energy variances. We then apply our results to a one-dimensional quantum walk, which is known to reproduce the Dirac equation in the small-mass and -momentum limit. We find that in this limit the effective IR dynamics is obtained by a mass redefinition.

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I. INTRODUCTION

Effective theories are a powerful and efficient way of organizing our description of physical processes [1–4]. The rough idea is that, in order to describe physical phenomena at some energy scale E, one does not need a full understanding of physics at much larger energy scales $\lambda \gg E$. The high-energy degrees of freedom approximately decouple, allowing one to describe the low-energy dynamics through an effective unitary theory. The only role of the high-energy degrees of freedom is to determine the parameters of this effective theory. The challenge of determining the effective theory has been studied for Hamiltonian dynamics, particularly within field theories [1–8]. However, the case of a system evolving in discrete time remains largely unexplored. The goal of this article is to help bridge this critical gap.

This kind of analysis is thus relevant for physical models such as quantum walks (QWs) [9–12] and quantum cellular automata (QCAs) [13–15]. QCAs and QWs are universal models of computation equivalent to the quantum circuit model [16,17]. In particular, QWs are interesting both as a quantum computing primitive, especially in search algorithms [9–12], and for quantum simulation [18–21]. QCAs describe quantum systems evolving under unitary and strictly local dynamics [22], so they can naturally be used for quantum simulations [23,24]. They are also the appropriate framework to handle Floquet systems [25]. It is natural to ask what kind of effective dynamics these models generate at large distances. More generally, discrete-time dynamics is a typical framework for quantum simulation, in which the target dynamics is obtained by Trotterization [26–31]. Therefore, one could be interested in what the effective dynamics of the simulator is when small-scale details of the implementation, which cannot be perfectly tuned, are traced out.

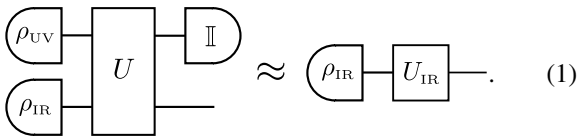
When we are interested in simulating quantum phenomena which are well described by some effective theory, we face two options. The first one is to directly simulate the effective theory on our quantum hardware (see, for example, [32–35]); the second one is to simulate a more fundamental theory known to reproduce the effective physics of interest at a large scale (see, for example, [36,37]). One advantage of this second approach is that by construction the quality of the simulation is largely insensitive to the details of the microscopic implementation, which is especially valuable for current pre-fault-tolerant quantum computers [38]. Typically, one can figure out a microscopic theory by time discretizing the target theory, recurring to Trotterization. This approach allows for a high degree of control since its approximation errors are well characterized [30,39]. On the other hand, if we rely on universality—i.e., the irrelevance of microscopic details to the large-scale behavior—it should be, in principle, possible to resort to a much simpler, yet highly effective, microscopic model. Therefore, there is room for simplification of implementations of a Trotterized model. Developing the tools to derive and analyze effective theories directly for discrete-time dynamics would be very valuable for validating the simplifications that one might consider.

Let us then consider a quantum system with Hilbert space $\mathcal{H}$ evolving in discrete steps by the repeated action of a unitary U. A qualitative difference from Hamiltonian dynamics is that, knowing only U, we do not have a well-defined notion

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of energy. We assume that the Hilbert space can be split between a fine-grained (UV) part and a coarse-grained (IR) part, $\mathcal{H} = \mathcal{H}_{\rm UV} \otimes \mathcal{H}_{\rm IR}$, of which we can observe only the latter. Then all the measurable phenomenology is determined by the IR reduced density matrix $\rho_{\rm IR} = {\rm Tr}_{\rm UV}\rho$, where ρ is the state of the whole system. In general, the dynamics in the IR sector of the theory is nonunitary because U produces entanglement between IR and UV degrees of freedom. We then address the following question: What is the unitary $U_{\rm IR}$ that best approximates the dynamics of the IR sector? In other words, our goal is finding the unitary $U_{\rm IR}$ such that



(1)

Once we know that $U_{\rm IR}$ is a good approximation of the dynamics at the scale of interest, we can use it in place of U. In other words, we generate the dynamics of the IR degrees of freedom by repeatedly applying $U_{\rm IR}$. Note that one can also look directly for an approximation of n time steps of the original theory, i.e., an approximation of U^n. This certainly results in a better approximation than applying n times the approximation of U. The benefit of allowing for a unitary approximation rather than using the exact nonunitary channel is that it simplifies both the analytical study and the simulation of the dynamics. At a more fundamental level, understanding which models of discrete dynamics lead to effectively unitary theories at long distances is important to understand whether they could be viable UV completion of known quantum field theories [40,41].

As a criterion to quantify the quality of the approximation we use the channel fidelity [42], a well-established measure of distinguishability between quantum channels. Moreover, this measure of distance is also justified by drawing a parallel with an analogous problem in the physics of open quantum systems. In this context, the UV degrees of freedom that we trace out can be viewed as an external environment, which we cannot control or observe. Open quantum systems evolve according to a master equation, which can be divided into a dissipative part and a Hamiltonian (or unitary) part. Although this division is not unique, it is typically chosen so that the dissipative term takes a Lindblad form. A recent work [43] showed that this seemingly *ad hoc* division corresponds to selecting the smallest possible dissipative term according to a metric that reduces to the channel fidelity when one of the channels is unitary. This approach was epitomized in Ref. [44] as the *principle of minimal dissipation*. From this perspective, we can say that the effective IR dynamics that we consider is the one minimizing dissipation.

Finding the best unitary $U_{\rm IR}$ by maximizing the channel fidelity is, in general, a challenging task, and we do not expect a good approximation to be achievable for arbitrary unitaries U. Therefore, we focus on the case in which the IR and UV degrees of freedom are weakly coupled. To leading order in the coupling, we show that the solution is a mean-field dynamics. We then apply this result to a QW on $\mathbb{Z}$, where the spatial lattice on which the walk takes place provides a natural way to split the Hilbert space between the UV and IR parts. Namely, we group the lattice points in bins: The IR degree of freedom specifies the bin in which the walker is located, and the UV degree of freedom specifies the position within the bin. In particular, we consider the Dirac QW from [45], which is known to reproduce the Dirac equation in the small-mass and large-wavelength limit. We find that in this same limit the effective dynamics is given by a simple rescaling of the mass that encapsulates all the dependence on the UV degrees of freedom.

Before continuing, we briefly point out previous works that have already considered the renormalization of systems evolving in discrete time steps. The question of how to renormalize QWs was considered in [46,47]. The main difference from our work is that in those works the authors renormalized the QW at the level of the generating function $\tilde{\psi}(x,z) = \sum_t \psi(x,t)z^t$, in which the explicit dependence on time is eliminated. Here, $\psi(x,t)$ is the wave function of the walker. Some form of coarse graining for QWs was also considered in [48] as part of an attempt to define discrete Lorentz invariance. Coarse graining of QCAs was considered in [49,50]. In [49], the authors considered a special type of QCA and implemented a coarse-graining procedure tailored for it. The prescription considered in this work should instead be generally applicable. In [50], the authors considered a general coarse-graining scheme for QCAs but imposed the requirement that the coarse-grained dynamics is *exactly* unitary. In this work, we consider the more general situation in which the coarse-grained dynamics is only approximately unitary.

The rest of this article is organized as follows. We begin by explaining our prescription for finding the effective IR dynamics. We then specialize to the case in which the UV and the IR are only weakly coupled and find the effective dynamics to leading order in this coupling. We apply this result to the Dirac QW on the line and find that when the coupling between UV and IR is weak, the coarse graining reduces to a mass renormalization. We conclude by pointing out some possible extensions of this work.

II. EFFECTIVE UNITARY DYNAMICS

Let us denote by $\rho = \rho_{\rm IR} \otimes \rho_{\rm UV}$ the initial state of the system, where $\rho_{\rm IR} \in \mathcal{L}(\mathcal{H}_{\rm IR})$ and $\rho_{\rm UV} \in \mathcal{L}(\mathcal{H}_{\rm UV})$. The channel describing the evolution of $\rho_{\rm IR}$ depends both on the specific system we consider and on $\rho_{\rm UV}$. We will keep $\rho_{\rm UV}$ generic and specify it only when we consider examples. If we had some notion of energy for the UV system, a reasonable choice would be to take $\rho_{\rm UV}$ to be the thermal state at some given temperature.

For a fixed $\rho_{\rm UV}$, the one-step evolution of the IR state $\rho_{\rm IR}$ is described by the channel $\mathcal{D}$, defined as follows:

$$\mathcal{D}(\rho_{\rm IR}) \coloneqq {\rm Tr}_{\rm UV}[U(\rho_{\rm IR} \otimes \rho_{\rm UV})U^\dagger]. \tag{2}$$

Our goal is to find the unitary channel $\mathcal{U}_{\rm IR}(\rho) \coloneqq U_{\rm IR}\rho U_{\rm IR}^\dagger$ which is as close as possible to the channel $\mathcal{D}$.

Let us consider the case in which the Hilbert space of the IR degrees of freedom is finite-dimensional, $d_{\rm IR} \coloneqq \dim \mathcal{H}_{\rm IR} < \infty$. The latter simplifying assumption can be justified by the fact that, in practice, only a finite number of degrees of freedom will be experimentally accessible. On formal grounds, this could be achieved by projecting down

to a finite-dimensional subspace of the original Hilbert space or considering periodic boundary conditions. As a measure of distance we use the channel fidelity $\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR})$ [42] between $\mathcal{D}$ and $\mathcal{U}_{\rm IR}$, which reads as follows:

$$\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) := \frac{1}{d_{\rm IR}^2} f(D, |U_{\rm IR}\rangle\!\rangle\langle\!\langle U_{\rm IR}|), \tag{3}$$

where $f(\rho,\sigma) := (\mathrm{Tr}\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}})^2$ is the state fidelity and D and $|U_{\rm IR}\rangle\!\rangle\langle\!\langle U_{\rm IR}|$ are the Choi operators [51] of channels $\mathcal{D}$ and $\mathcal{U}_{\rm IR}$, given by $D = (\mathcal{D}\otimes\mathcal{I})(|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|)$ and $|U_{\rm IR}\rangle\!\rangle = (U_{\rm IR}\otimes\mathbb{1})|\mathbb{1}\rangle\!\rangle$. Here, we use the notation $|A\rangle\!\rangle := \sum_{i,j=1}^{d_{\rm IR}} A_{i,j}|i\rangle|j\rangle$ for an operator $A = \sum_{i,j=1}^{d_{\rm IR}} A_{i,j}|i\rangle\langle j|$. If, as in our case, one of the two channels is unitary, the channel fidelity can be expressed as the average of the state fidelity over pure input states, i.e., $d_{\rm IR}\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) = (d_{\rm IR}+1)\int d\psi\,\langle\psi|U_{\rm IR}^\dagger\mathcal{D}(|\psi\rangle\langle\psi|)U_{\rm IR}|\psi\rangle - 1$, where $d\psi$ is the Haar measure of the group $\mathrm{SU}(d_{\rm IR})$. This criterion also coincides with the one used in Refs. [43,44] to assess the distance between dissipative superoperators. By inserting Eq. (2) into Eq. (3) we obtain

$$\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) = \frac{1}{d_{\rm IR}^2}\mathrm{Tr}_{\rm UV}[O_{\rm UV}\rho_{\rm UV}O_{\rm UV}^\dagger], \tag{4}$$

$$O_{\rm UV} := \mathrm{Tr}_{\rm IR}[(U_{\rm IR}^\dagger\otimes\mathbb{1}_{\rm UV})U]. \tag{5}$$

We note that the quantity we want to maximize is invariant under $O_{\rm UV}\to VO_{\rm UV}$ for any unitary V.

Clearly, when the dynamics factorizes as $U = V_{\rm IR}\otimes V_{\rm UV}$, the maximum value $\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) = 1$ is simply achieved by taking $U_{\rm IR} = V_{\rm IR}$. On the other hand, it is worth noting that the condition $\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) = 1$ does not necessarily imply that U factorizes; an easy counterexample is a controlled unitary $U = U_{\rm IR}^0\otimes|0\rangle\langle 0| + U_{\rm IR}^1\otimes|1\rangle\langle 1|$ with $\rho_{\rm UV} := |0\rangle\langle 0|$. However, if $\rho_{\rm UV}$ has full rank, then $\mathcal{F}(\mathcal{D},\mathcal{U}_{\rm IR}) = 1$ does imply that the evolution U factorizes [52].

III. WEAKLY COUPLED IR AND UV

The effective unitary dynamics will generally be a poor approximation for most choices of U. For instance, a Haar-random unitary typically generates maximal entanglement between UV and IR degrees of freedom even after a single step. However, many physical theories possess additional structures, such as locality and symmetries, that set them apart from a typical Haar-random unitary. From the discussion above, we understand that unitaries allowing for a well-approximated effective unitary dynamics are those that approximately factorize.

Therefore, we now specialize to this case and consider

$$U = (V_{\rm IR}\otimes V_{\rm UV})U_{\rm MIX}(\theta), \tag{6}$$

where $U_{\rm MIX}(\theta)$ is analytic at $\theta = 0$, with $U_{\rm MIX}(0) = \mathbb{1}$. Then UV and IR are weakly coupled when $\theta \ll 1$. The condition of weak IR-UV coupling is far from artificial; for example, it is satisfied in quantum field theory when one wants to find the effective dynamics of some light field weakly coupled to a heavy field [1–3,53]. Below we will show that it is also applicable to an interesting example of a quantum walk. Note that the parameter θ is introduced as an abstract parameter that guarantees that the dynamics approximately factorizes for $\theta \ll 1$. Its physical interpretation is model dependent. For example, in the Dirac quantum walk θ turns out to be the mass. If $U_{\rm MIX}$ were generated by a Hamiltonian λV, then θ would be equal to λ times the time step.

We now proceed to find $U_{\rm IR}$ to leading order in θ. Due to the invariance of $\mathcal{F}$ under $O_{\rm UV}\to VO_{\rm UV}$, we can safely ignore $V_{\rm UV}$. Then we have $O_{\rm UV} = \mathrm{Tr}_{\rm IR}[(U_{\rm IR}^\dagger V_{\rm IR}\otimes\mathbb{1}_{\rm UV})U_{\rm MIX}(\theta)]$, and from the discussion above, it is clear that $U_{\rm IR}^\dagger V_{\rm IR}$ goes to the identity for $\theta\to 0$. This suggests expanding both $U_{\rm MIX}$ and $V_{\rm IR}^\dagger U_{\rm IR}$ in a Taylor expansion in θ and determining $\mathcal{F}$ order by order. Namely, let

$$\begin{aligned} U_{\rm MIX} &= \mathbb{1} + i\theta H_{\rm MIX} + \theta^2 L_{\rm MIX} + O(\theta^3),\\ V_{\rm IR}^\dagger U_{\rm IR} &= \mathbb{1} + i\theta H_{\rm IR} + \theta^2 L_{\rm IR} + O(\theta^3). \end{aligned} \tag{7}$$

Unitarity implies that $H_{\rm MIX} = H_{\rm MIX}^\dagger$ and $L_{\rm MIX} + L_{\rm MIX}^\dagger = -H_{\rm MIX}^2$, and similar relations for $H_{\rm IR}$ and $L_{\rm IR}$. Plugging these two expansions in (4), we find

$$\mathcal{F} = 1 - \theta^2\left\langle \mathrm{Tr}_{\rm IR}\frac{\Delta^2}{d_{\rm IR}} - \left(\mathrm{Tr}_{\rm IR}\frac{\Delta}{d_{\rm IR}}\right)^2\right\rangle_{\rm UV} + O(\theta^3), \tag{8}$$

where $\langle\cdot\rangle_{\rm UV} = \mathrm{Tr}_{\rm UV}[\rho_{\rm UV}\cdot]$, $\langle\cdot\rangle_{\rm IR} = \mathrm{Tr}_{\rm IR}[\cdot]/d_{\rm IR}$, and $\Delta = H_{\rm MIX} - H_{\rm IR}\otimes\mathbb{1}_{\rm UV}$. We can show that the term in the angle brackets is negative, as it should be since we know that the whole quantity is upper bounded by 1. Some algebra shows that the expression above for $\mathcal{F}$ is equivalent to

$$\begin{aligned} \mathcal{F} &= 1 - \theta^2\big[\langle\delta^2\rangle_{\rm IR} - \langle\delta\rangle_{\rm IR}^2 + \mu(H_{\rm MIX})\big] + O(\theta^3),\\ \delta &:= H_{\rm IR} - \mathrm{Tr}_{\rm UV}[(\rho_{\rm UV}\otimes\mathbb{1}_{\rm IR})H_{\rm MIX}], \end{aligned} \tag{9}$$

where

$$\begin{aligned} \mu(H_{\rm MIX}) :=& \mathrm{Tr}_{\rm UV}\left[\rho_{\rm UV}\mathrm{Tr}_{\rm IR}\frac{H_{\rm MIX}^2}{d_{\rm IR}}\right]\\ &- \mathrm{Tr}_{\rm UV}\left[\rho_{\rm UV}\left(\mathrm{Tr}_{\rm IR}\frac{H_{\rm MIX}}{d_{\rm IR}}\right)^2\right]\\ &- \frac{1}{d_{\rm IR}}\mathrm{Tr}_{\rm IR}(\mathrm{Tr}_{\rm UV}[\rho_{\rm UV}\otimes\mathbb{1}_{\rm IR}\cdot H_{\rm MIX}])^2\\ &+ \frac{1}{d_{\rm IR}^2}(\mathrm{Tr}_{\rm UV}[\rho_{\rm UV}\mathrm{Tr}_{\rm IR}H_{\rm MIX}])^2. \end{aligned} \tag{10}$$

For the moment, the important point is that μ does not depend on $H_{\rm IR}$.

The first two terms in the brackets on the right-hand side of Eq. (9) instead do depend on $H_{\rm IR}$ and are clearly non-negative, so $\mathcal{F}$ is maximized when $\delta = 0$, which fixes $H_{\rm IR}$. Exponentiating $H_{\rm IR}$ to make sure that $U_{\rm IR}$ is unitary, we find

$$U_{\rm IR} = V_{\rm IR}e^{i\theta H_{\rm IR}}, \quad H_{\rm IR} = \mathrm{Tr}_{\rm UV}[(\rho_{\rm UV}\otimes\mathbb{1}_{\rm IR})H_{\rm MIX}]. \tag{11}$$

We conclude that the best unitary approximation for the IR dynamics is obtained by taking $H_{\rm IR}$ as a mean-field average over $\rho_{\rm UV}$.

To leading order, we also know the error introduced by the unitarity constraint, i.e., μ. If we decompose the mixing operator as

$$H_{\rm MIX} = \sum_{\lambda=0}^{d_{\rm IR}^2-1} H_{{\rm UV},\lambda}\otimes H_{{\rm IR},\lambda}, \tag{12}$$

where $\{H_{\mathrm{IR},\lambda}\}_{\lambda=0}^{d_{\mathrm{IR}}^2-1}$ is a basis of the space of the Hermitian operator on $\mathcal{H}_{\mathrm{IR}}$, and define the connected correlator as $\langle AB\rangle^c = \langle AB\rangle - \langle A\rangle\langle B\rangle$, where $\langle A\rangle = \mathrm{Tr}[A\rho]$, we have

$$\mu = \sum_{\lambda\lambda'} \langle H_{\mathrm{IR},\lambda} H_{\mathrm{IR},\lambda'}\rangle_{\mathrm{IR}}^c \langle H_{\mathrm{UV},\lambda} H_{\mathrm{UV},\lambda'}\rangle_{\mathrm{UV}}^c. \tag{13}$$

We can further simplify this expression if we choose a basis such that $H_{\mathrm{IR},0} = \mathbb{1}_{\mathrm{IR}}$ and $\mathrm{Tr}[H_{\mathrm{IR},\lambda} H_{\mathrm{IR},\lambda'}] = d_{\mathrm{IR}}\delta_{\lambda,\lambda'}$. In this basis, we find $\langle H_{\mathrm{IR},\lambda} H_{\mathrm{IR},\lambda'}\rangle_{\mathrm{IR}}^c = 1$ if $\lambda = \lambda' \neq 0$ and 0 otherwise, and μ becomes

$$\mu = \sum_{\lambda\neq 0} \left\langle H_{\mathrm{UV},\lambda}^2 \right\rangle_{\mathrm{UV}}^c. \tag{14}$$

This is simply the sum of energy variances in ρ_{UV}. Putting everything together, we find that the best achievable $\mathcal{F}$ is

$$\mathcal{F} = 1 - \theta^2 \sum_{\lambda\neq 0} \left\langle H_{\mathrm{UV},\lambda}^2 \right\rangle_{\mathrm{UV}}^c + O(\theta^3), \tag{15}$$

where the UV Hamiltonians are defined by decomposing H_{MIX} as explained above. Note that the leading-order error can be trusted only when $\theta \ll 1$.

IV. EFFECTIVE DYNAMICS OF THE DIRAC QW

In this section, we apply our prescription to a one-dimensional discrete-time quantum walk given by the unitary operator

$$U = \begin{pmatrix} \cos(\theta)\, T^\dagger & -i\sin(\theta) \\ -i\sin(\theta) & \cos(\theta)\, T \end{pmatrix}, \quad U \in \mathcal{L}(l_2(\mathbb{Z}) \otimes \mathbb{C}^2), \tag{16}$$

where T is the translation operator, which acts on the position basis as $T|x\rangle = |x-1\rangle$, and $\theta \in [0, \pi/4]$ is the only free parameter of the theory. The update rule is local; i.e., $\psi(x,t)$ depends on only $\psi(y, t-1)$ for $y \in \{x-1, x, x+1\}$. So this model has a strict light cone; i.e., at each time step information propagates at most by one lattice point. This model is known to reproduce the Dirac equation in one dimension in the limit of small momenta [45], and for this reason it is called the Dirac QW. Given the translational symmetry of the system, it is convenient to work in momentum space, and the walk operator becomes $U = \int_{2\pi} U(p) \otimes |p\rangle\langle p| dp$, where

$$U(p) = \begin{pmatrix} e^{ip}\cos(\theta) & -i\sin(\theta) \\ -i\sin(\theta) & e^{-ip}\cos(\theta) \end{pmatrix}. \tag{17}$$

The lattice suggests a simple way of coarse graining the Hilbert space. We group the sites of the lattice in pairs and relabel positions by two indices: The first specifies the bin, and the second specifies the position inside the bin, namely,

$$|x\rangle = |x_{\mathrm{IR}}\rangle \otimes |x_{\mathrm{UV}}\rangle, \tag{18}$$

where $x_{\mathrm{IR}} = \lfloor x/2 \rfloor \in \mathbb{Z}$ and $x_{\mathrm{UV}} = (x \mod 2) \in \{0, 1\}$, such that $x = 2x_{\mathrm{IR}} + x_{\mathrm{UV}}$ (see Fig. 1). The total Hilbert space $\mathcal{H}$ is then factorized as $\mathcal{H} = \mathcal{H}_{\mathrm{IR}} \otimes \mathcal{H}_{\mathrm{UV}}$, where $\mathcal{H}_{\mathrm{IR}} = l_2(\mathbb{Z}) \otimes \mathbb{C}^2$ tracks the bin and the internal degree of freedom (DOF) of the walker, while $\mathcal{H}_{\mathrm{UV}} = \mathbb{C}^2$ keeps track of whether the walker is on an even or odd site within the bin. Correspondingly, in momentum space $|p\rangle = (2\pi)^{-1/2} \sum_x e^{-ipx}|x\rangle$, we have

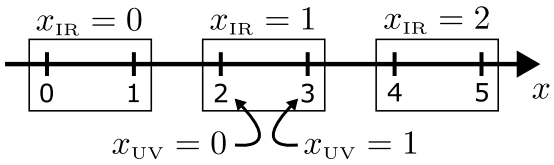


FIG. 1. Coarse-graining procedure for a QW on $\mathbb{Z}$.

$$|p\rangle = |2p\rangle_{\mathrm{IR}} \otimes (|0\rangle_{\mathrm{UV}} + e^{-ip}|1\rangle_{\mathrm{UV}}), \tag{19}$$

where in the parentheses $|0\rangle_{\mathrm{UV}}$ and $|1\rangle_{\mathrm{UV}}$ are the UV position basis eigenstates.

We will accompany the spatial coarse graining with a temporal one. The motivation is twofold. On the one hand, if we assume some experimental limitations on the spatial resolution, it seems reasonable to assume that similar limitations will hold for the temporal resolution of measurements. On the other hand, this guarantees that the coarse graining preserves the light cone. A rather straightforward calculation gives $U^2 = (V_{\mathrm{IR}} \otimes V_{\mathrm{UV}}) U_{\mathrm{MIX}}(\theta)$, where

$$V_{\mathrm{IR}} = \begin{pmatrix} T_{\mathrm{IR}}^\dagger & 0 \\ 0 & T_{\mathrm{IR}} \end{pmatrix}, \quad V_{\mathrm{UV}} = I, \tag{20}$$

T_{IR} is the translation operator on $\mathcal{H}_{\mathrm{IR}}$, and $U_{\mathrm{MIX}}(\theta)$ is a unitary operator such that $U_{\mathrm{MIX}}(0) = \mathbb{1}$. Then, in the limit of interest, i.e., $\theta \ll 1$, U^2 approximately factorizes, and we can apply Eq. (11). Note that in this case, $\mathcal{H}_{\mathrm{IR}}$ has infinite dimensions, so we will technically be beyond the validity of the result in the previous section. We could circumvent this problem by placing the walk on a finite, but sufficiently long, chain with periodic boundary conditions. This is equivalent to restricting the set of allowed observables to those with sufficiently small support. In any case, the formally infinite factors of d_{IR} cancel in the formula for the mean field effective unitary, so to avoid cluttering the notation we keep the walk on $\mathbb{Z}$. In Appendix B, we repeat the calculations in this section on a finite ring and check that the result is indeed the same.

As a first step we split U^2 into the product of one term which can trivially coarse grained and one term that goes to the identity in the $\theta \to 0$ limit. Namely, $U^2 = (\mathbb{1}_{\mathrm{UV}} \otimes V_{\mathrm{IR}}) \cdot U_{\mathrm{MIX}}$, where

$$V_{\mathrm{IR}} = \begin{pmatrix} T_{\mathrm{IR}}^\dagger & 0 \\ 0 & T_{\mathrm{IR}} \end{pmatrix}, \quad U_{\mathrm{MIX}} = \begin{pmatrix} A & -iB \\ -iB^\dagger & A^\dagger \end{pmatrix}, \tag{21}$$

with $A \coloneqq \cos^2(\theta)\mathbb{1} - \sin^2(\theta)T^2$ and $B \coloneqq \sin(\theta)\cos(\theta)(T + T^\dagger)T^2$. Since U_{MIX} is analytic as a function of θ and $U_{\mathrm{MIX}} \to \mathbb{1}$ for $\theta \to 0$, we can apply (11). Taking the derivative of U_{MIX} and setting $\theta = 0$, we find that $H_{\mathrm{MIX}} = \int_{2\pi} H_{\mathrm{MIX}}(p) \otimes |p\rangle\langle p| dp$, with

$$H_{\mathrm{MIX}}(p) = -2\cos(p) \begin{pmatrix} 0 & e^{-i2p} \\ e^{2ip} & 0 \end{pmatrix}. \tag{22}$$

To compute $H_{\mathrm{IR}} = \mathrm{Tr}_{\mathrm{UV}}[\rho_{\mathrm{UV}} \otimes \mathbb{1}_{\mathrm{IR}} \cdot H_{\mathrm{MIX}}]$, we use

$$|p\rangle\langle p| = \begin{pmatrix} 1 & e^{ip} \\ e^{-ip} & 1 \end{pmatrix}_{\mathrm{UV}} \otimes |2p\rangle\langle 2p|_{\mathrm{IR}} \tag{23}$$

and paramatrize $\rho_{\rm UV} = (\mathbb{1} + r_x\sigma_x + r_y\sigma_y + r_z\sigma_z)/2$. We find that

$$\mathrm{Tr}_{\rm UV}[\rho_{\rm UV}\cdot|p\rangle\langle p|] = [1 + r_{xy}(p)]|2p\rangle\langle 2p|_{\rm IR}, \tag{24}$$

where $r_{xy}(p) \coloneqq r_x\cos(p) - r_y\sin(p)$. Using this, we find

$$H_{\rm IR} = -2\int_{-\pi}^{\pi}[1 + r_{xy}(p)]\cos(p)\begin{pmatrix}0 & e^{-i2p}\\ e^{i2p} & 0\end{pmatrix}\otimes|2p\rangle\langle 2p|_{\rm IR}.$$

Rescaling the integral $p \to p/2$ and using $|p \pm 2\pi\rangle = |p\rangle$, we can rewrite the integral as follows:

$$H_{\rm IR} = \gamma(p)\begin{pmatrix}0 & e^{-ip}\\ e^{ip} & 0\end{pmatrix}\otimes|p\rangle\langle p|_{\rm IR}, \tag{25}$$

$$\gamma(p) \coloneqq r_x[1 + \cos(p)] - r_y\sin(p). \tag{26}$$

Exponentiating $H_{\rm IR}$ and multiplying by $V_{\rm IR}$, we obtain $U_{\rm IR} = \int_{2\pi} U_{\rm IR}(p)\otimes|p\rangle\langle p|_{\rm IR}dp$,

$$U_{\rm IR}(p) = \begin{pmatrix}e^{ip}\cos[\gamma(p)\theta] & -i\sin[\gamma(p)\theta]\\ -i\sin[\gamma(p)\theta] & e^{-ip}\cos[\gamma(p)\theta]\end{pmatrix},$$

$$\gamma(p) \coloneqq r_x([1 + \cos(p)] - r_y\sin(p). \tag{27}$$

Note that all the dependence on UV data is contained in $\gamma(p)$.

Comparing Eq. (27) and (17), we notice that the functional shape is the same, but the mass term is now dependent on p, $\theta \to \gamma(p)\theta$. The dispersion relation, which originally was $\cos[\omega(p)] = \cos(p)\cos(\theta)$, is now $\cos[\omega_{\rm IR}(p)] = \cos(p)\cos[\gamma(p)\theta]$. The comparison further simplifies if we consider the small-momentum regime, i.e., $p \to 0$. To leading order we have $\cos[\omega(p)] = 1 - p^2/2 - \theta^2/2$ and $\cos[\omega_{\rm IR}(p)] = 1 - p^2/2 - 2\theta^2 r_x^2$, and in this limit the effective dynamics is obtained with a simple rescaling, $\theta \to 2\theta r_x$.

To quantify the error introduced by this unitary approximation, we can use (13). First, we decompose $H_{\rm MIX}$ as $H_{\rm MIX} = \int_{2\pi} H_{\rm UV}(p)\otimes H_{\rm IR}(p)\,dp$, with

$$H_{\rm UV}(p) = -2\cos(p/2)\begin{pmatrix}0 & e^{ip/2}\\ e^{-ip/2} & 0\end{pmatrix} \tag{28}$$

and

$$H_{\rm IR}(p) = \begin{pmatrix}0 & e^{-ip}\\ e^{ip} & 0\end{pmatrix}\otimes|p\rangle\langle p|_{\rm IR}. \tag{29}$$

How to compute the trace over the IR DOF is not exactly clear because the number of IR DOF is formally infinite. In particular, we need to give a prescription for dealing with expressions such as $\mathrm{Tr}_{\rm IR}[|p\rangle\langle p|_{\rm IR}]/d_{\rm IR} \propto (\sum_{x_{\rm IR}} 1)/d_{\rm IR}$, where both $d_{\rm IR}$ and the sum are formally infinite. We can deal with this type of expressions by putting everything in a box, i.e., considering a closed chain of size $4L$. Then after coarse graining, we are left with $2L$ sites. Taking into account the coin DOF as well, we have $d_{\rm IR} = 4L$, and $\sum_{x_{\rm IR}} 1 = 2L$, so the two infinities cancel out, and we are left with $\mathrm{Tr}_{\rm IR}[|p\rangle\langle p|_{\rm IR}]/d_{\rm IR} = 4\pi$. Using this, we find that

$$\begin{aligned}\langle H_{\rm UV}(p)\rangle &= 2\cos(p/2)[r_x\cos(p/2) - r_y\sin(p/2)],\\ \langle H_{\rm UV}(p)H_{\rm UV}(q)\rangle &= 4\cos(p/2)\cos(q/2)\\ &\quad\times\left(\cos\frac{p-q}{2} - r_z\sin\frac{p-q}{2}\right),\\ \langle H_{\rm IR}(p)\rangle &= 0, \quad \langle H_{\rm IR}(p)H_{\rm IR}(q)\rangle = \frac{1}{2\pi}\delta(p-q),\end{aligned} \tag{30}$$

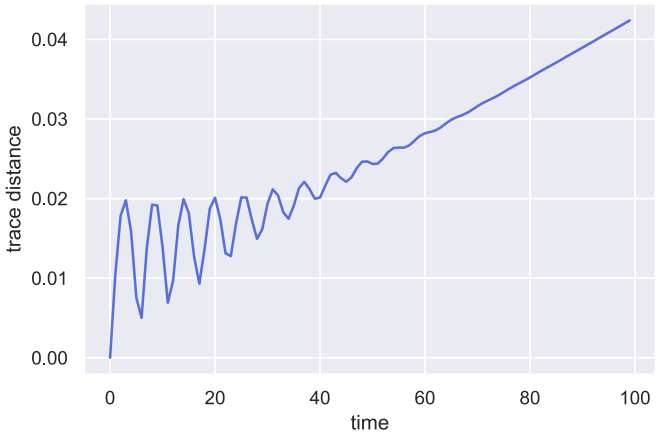


FIG. 2. Trace distance between coarse-grained dynamics and exact dynamics as a function of time for the propagation of a Gaussian packet.

which leads to

$$\mu = \tfrac{1}{2}\left(4 - 3r_x^2 - r_y^2\right). \tag{31}$$

Note that the error is minimized for $r_x = 1$, which corresponds to $\rho_{\rm UV} = |+\rangle\langle+|$, with $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, and that no choice of $\rho_{\rm UV}$ can make this error vanish.

We numerically check the validity of the unitary approximation by numerically simulating the propagation of a Gaussian packet. The result is displayed in Fig. 2. After a transient regime with some oscillations, we see that the error grows linearly due to the accumulation of the small error made at each step of the evolution.

V. CONCLUSION

In this work, we considered the question of whether the coarse-grained dynamics of a quantum system evolving discretely in time can be effectively described by a unitary theory. We introduced a prescription for finding the best unitary approximation of the IR dynamics by maximizing the channel fidelity. Physically, this can be interpreted as minimizing dissipation to the unobserved UV DOF. When the UV and IR degrees of freedom were weakly coupled, we carried out the maximization to leading order in the coupling constant, and we found that the best unitary effective dynamics is given by a mean-field-like average over the UV DOF, Eq. (11). Our result agrees with the one found in the same regime but for continuous time evolution in [53]. We also showed that the error in the approximation can be expressed as a sum of energy variances, (14). We then applied these results to the Dirac QW in the limit of small masses, $\theta \ll 1$, and small momenta. We found that the effect of the coarse graining is to renormalize the mass, and we checked that the coarse-graining leads to a good approximation by numerically simulating the QW with Gaussian wave packets.

There are several ways in which the present work could be further extended. A natural extension would be to consider other QWs and check whether, at least in some limit, the coarse graining reduces to the renormalization of some of the parameters of the walker, like what happened for the

Dirac QW. In particular, it would be interesting to consider interacting QWs (e.g., [54,55]) and see how the coarse-graining procedure affects the coupling constant. In this work we assumed that the Hilbert space can be simply factorized between UV and IR degrees of freedom as $\mathcal{H} = \mathcal{H}_{\rm IR} \otimes \mathcal{H}_{\rm UV}$ and that the coarse graining corresponds to tracing out the UV degrees of freedom. It would be interesting to relax both these assumptions, the first because it is not always possible to exactly factorize the Hilbert space between UV and IR degrees of freedom and the second because IR observables do not necessarily act as the identity on the UV. In other words, it would be interesting to consider more sophisticated ways of splitting the Hilbert space between IR and UV degrees of freedom and more sophisticated coarse-graining procedures. We think that a good starting point along this path are Refs. [56–58].

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DATA AVAILABILITY

The data that support the findings of this article are openly available [59].

APPENDIX A: NUMERICS DETAILS

We provide some further details on the numerics performed to generate Fig. 2. To simulate the QW we consider a closed chain of size $2L = 2000$, and we pick $\theta = 0.2$. The Gaussian packet is given by

$$|\psi_{\sigma_k,k_0,x_0}\rangle := \int_{-\pi}^{\pi} dk\, \psi_{\sigma_k,k_0,x_0}(k)|w_+(k)\rangle \otimes |k\rangle,$$
$$\psi_{\sigma_k,k_0,x_0}(k) := \frac{1}{N_{\sigma_k,k_0}} \exp\left[-\frac{(k-k_0)^2}{2\sigma_k^2} + ikx_0 \right]. \quad \text{(A1)}$$

Here, $|w_\pm(k)\rangle$ are the eigenvectors of (16), which are given by [55]

$$|w_\pm(p)\rangle = \frac{1}{M_\pm(p)} \begin{pmatrix} -i\sin(\theta) \\ h_\pm(p) \end{pmatrix},$$
$$h_\pm(p) := -i[\pm \sin\omega(p) + \cos(\theta)\sin(p)], \quad \text{(A2)}$$

with $\omega(p) := \arccos[\cos(\theta)\cos(p)]$ and $M_\pm(p)^2 := \cos(\theta)^2 + |h_\pm(p)|^2$. Before continuing to consider the numerical simulation, we explain some properties of this state.

We are interested in the $\sigma_k \ll 1$ regime, for which, as we see below, the wave function changes sufficiently slowly in the position basis that the state is approximately factorized between UV and IR. In this regime, we can evaluate the integral over k by a saddle approximation and find that in the position basis the packet looks like

$$|\psi_{\sigma_k,k_0,x_0}\rangle \approx |w_+(k_0)\rangle \otimes |\phi\rangle,$$
$$|\phi\rangle := \sum_x \exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2} - ik_0(x-x_0) \right] |x\rangle, \quad \text{(A3)}$$

where $\sigma_x = 1/\sigma_k$ and we have omitted the normalization. Let us focus on $|\phi\rangle$. Under the mapping $|x\rangle \to |x_{\rm IR}\rangle \otimes |x_{\rm UV}\rangle$, it becomes

$$|\phi\rangle = \sum_{x_{\rm IR}} \left\{ \exp\left[-\frac{2(x_{\rm IR} - x_{{\rm IR},0})^2}{\sigma_x^2} \right] e^{-i2k_0(x_{\rm IR} - x_{{\rm IR},0})} |x_{\rm IR}\rangle \right.$$
$$\otimes \sum_{x_{\rm UV}} \exp\left[-\frac{2(x_{\rm IR} - x_{{\rm IR},0})(x_{\rm UV} - x_{{\rm UV},0})}{\sigma_x^2} \right.$$
$$\left. \left. - \frac{(x_{\rm UV} - x_{{\rm UV},0})^2}{2\sigma_x^2} \right] \right.$$
$$\left. \times\, e^{-ik_0(x_{\rm UV} - x_{{\rm UV},0})} |x_{\rm UV}\rangle \right\}, \quad \text{(A4)}$$

where we have set $x_0 = 2x_{{\rm IR},0} + x_{{\rm UV},0}$. For $\sigma_x \gg 1$ we can drop the first exponential inside the sum over $x_{\rm UV}$, and we find that $|\phi\rangle$ approximately factorizes. Moreover, the UV state is $\rho_{\rm UV} = |\phi_{\rm UV}\rangle\langle\phi_{\rm UV}|$, with

$$|\phi_{\rm UV}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{-ik_0}|1\rangle). \quad \text{(A5)}$$

Note that here, we have dropped an irrelevant phase depending on $x_{{\rm UV},0}$. From the analysis in the main text, we know that in the limit of small momenta all we need to do is renormalize the mass $\theta \to 2\theta r_x$, and for the states above $r_x = \cos k_0$.

In Fig. 2, we plot the trace distance between the IR density matrix obtained by either evolving and then tracing or first tracing and evolving with $U_{\rm IR}$, i.e.,

$$\mathcal{E}_n = \tfrac{1}{2} \left\| {\rm Tr}_{\rm UV}[U^{2n}\rho(U^\dagger)^{2n}] - U_{\rm IR}^n \rho_{\rm IR} (U_{\rm IR}^\dagger)^n \right\|_1. \quad \text{(A6)}$$

The plot is generated for a Gaussian wave packet with $\sigma_k = 0.02$, $k_0 = 0.2$, and $x_0 = -200$.

APPENDIX B: QW IN A BOX

We rederive the effective dynamics for the Dirac quantum walk in the main text, regularizing the IR by putting it in a box. Namely, we now consider a QW on a closed chain of size $4L$. The Hilbert space is spanned by $|x\rangle$ for $x = 0, 1, \ldots, 4L-1$, and $|x = 4L\rangle \equiv |x = 0\rangle$. Momentum eigenstates are now

$$|p\rangle = \frac{1}{\sqrt{4L}} \sum_{x=0}^{4L-1} e^{-i\frac{\pi p}{2L}x} |x\rangle, \quad p \in \mathbb{Z}, \quad \text{(B1)}$$

and $|p\rangle = |p + 4L\rangle$. We take as the first Brillouin zone $p \in [-2L, 2L-1]$. The coarse graining corresponds to

$$|p\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_{\rm UV} + e^{-i\frac{\pi p}{2L}}|1\rangle_{\rm UV}\right) \otimes |p\rangle_{\rm IR}, \quad \text{(B2)}$$

with

$$|p\rangle_{\rm IR} = \frac{1}{\sqrt{2L}} \sum_{x_{\rm IR}=0}^{2L-1} e^{-i\frac{\pi p}{L}x_{\rm IR}} |x_{\rm IR}\rangle_{\rm IR}, \quad p \in \mathbb{Z}, \tag{B3}$$

where $x_{\rm IR} = 0, 1, \ldots, 2L-1$ and $|p\rangle_{\rm IR} = |p+2L\rangle_{\rm IR}$. We take as the first Brillouin zone $p \in [-L, L-1]$.

Following the same steps as for the infinite case, we find that

$$H_{\rm MIX} = -2 \sum_{p=-2L}^{2L} \cos\left(\frac{\pi p}{2L}\right) \begin{pmatrix} 0 & e^{-i\frac{\pi p}{L}} \\ e^{i\frac{\pi p}{L}} & 0 \end{pmatrix} \otimes |p\rangle\langle p|. \tag{B4}$$

Using (B2) and rearranging the summation indices, we arrive at

$$H_{\rm MIX} = -2 \sum_{p=-L}^{L-1} \cos\left(\frac{\pi p}{2L}\right) \begin{pmatrix} 0 & e^{-i\frac{\pi p}{2L}} \\ e^{i\frac{\pi p}{2L}} & 0 \end{pmatrix}_{\rm UV} \otimes \begin{pmatrix} 0 & e^{-i\frac{\pi p}{L}} \\ e^{i\frac{\pi p}{L}} & 0 \end{pmatrix}_{c} \otimes |p\rangle\langle p|_{\rm IR}, \tag{B5}$$

where the subscript c denotes the coin factor. Computing $H_{\rm IR} = {\rm Tr}_{\rm UV}[\rho_{\rm UV} \otimes \mathbb{1}_{\rm IR} \cdot H_{\rm MIX}]$, we find

$$H_{\rm IR} = -i \sum_{p=-L}^{L-1} r_{xy}(p) \begin{pmatrix} 0 & e^{-i\frac{\pi p}{L}} \\ e^{i\frac{\pi p}{L}} & 0 \end{pmatrix}_{c} \otimes |p\rangle\langle p|_{\rm IR},$$
$$r_{xy}(p) := r_x\left(1 + \cos\frac{\pi p}{L}\right) - r_y \sin\frac{\pi p}{L}. \tag{B6}$$

From here on the calculation follows identically that of the infinite case, and we find $\theta_{\rm IR}(p) = \{r_x[1+\cos(\pi p/L)] - r_y \sin(\pi p/L)\}\theta$.

To compute μ we parametrize $\rho_{\rm UV}$ as explained in the main text, and we take $\rho_{\rm IR} = \mathbb{1}_{\rm IR}/d_{\rm IR}$, which is now well-defined with $d_{\rm IR} = 4L$ (which includes a factor of 2 for the coin space). To compute μ using Eq. (10), we find

$$\begin{aligned} &{\rm Tr}_{\rm UV}\left[\rho_{\rm UV} {\rm Tr}_{\rm IR} \frac{H_{\rm MIX}^2}{d_{\rm IR}}\right] = -\frac{2}{L}\sum_{p=-L}^{L-1} \cos^2\left(\frac{\pi p}{2L}\right), \\ &{\rm Tr}_{\rm UV}\left[\rho_{\rm UV}\left({\rm Tr}_{\rm IR}\frac{H_{\rm MIX}}{d_{\rm IR}}\right)^2\right] = 0, \\ &\frac{1}{d_{\rm IR}}{\rm Tr}_{\rm IR}({\rm Tr}_{\rm UV}[\rho_{\rm UV}\otimes\mathbb{1}_{\rm IR}\cdot H_{\rm MIX}])^2 = \frac{-1}{2L}\sum_{p=-L}^{L-1} r_{xy}^2(p), \\ &\frac{1}{d_{\rm IR}^2}({\rm Tr}_{\rm UV}[\rho_{\rm UV}{\rm Tr}_{\rm IR}H_{\rm MIX}])^2 = 0. \end{aligned} \tag{B7}$$

The sums above can be calculated analytically,

$$\begin{aligned} \frac{2}{L}\sum_{p=-L}^{L-1}\cos^2\left(\frac{\pi p}{2L}\right) &= 2, \\ \frac{1}{2L}\sum_{p=-L}^{L-1} r_{xy}^2(p) &= \frac{1}{2}\left(3r_x^2 + r_y^2\right). \end{aligned} \tag{B8}$$

So, finally, we arrive again at (31).

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