

Scattering and Perturbation Theory for Discrete-Time Dynamics

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We present a systematic treatment of scattering processes for quantum systems whose time evolution is discrete. We define and show some general properties of the scattering operator, in particular the conservation of quasienergy which is defined only modulo 2π . Then we develop two perturbative techniques for the power series expansion of the scattering operator, the first one analogous to the iterative solution of the Lippmann-Schwinger equation, the second one to the Dyson series of perturbative quantum field theory. We use this formalism to compare the scattering amplitudes of a continuous-time model and of the corresponding discretized one. We give a rigorous assessment of the comparison for the case of bounded free Hamiltonian, as in a lattice theory with a bounded number of particles. Our framework can be applied to a wide class of quantum simulators, like quantum walks and quantum cellular automata. As a case study, we analyze the scattering properties of a one-dimensional cellular automaton with locally interacting fermions.

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Introduction.—Simulation of the time evolution of an arbitrary quantum system on a classical computer is a computationally hard task. In one of the seminal papers of quantum computation [1], Feynman suggested that this problem could be evaded by having a quantum system simulate another one. This intuition was proved to be correct [2]: a quantum computer (or universal quantum simulator) can indeed efficiently simulate any quantum system evolving through local interactions.

In recent years, there has been an increasing interest in quantum simulators, with a broad range of theoretical proposals (see, e.g., Refs. [3–10] and the reviews [11,12]), as well as various experimental proofs of concept [13–17].

Except for selected cases where the dynamics of the system can be mapped into the dynamics of the simulator (e.g., in the trapped ion simulation of the Dirac equation [18]), one has to engineer a discrete quantum model of the system to be simulated. The most studied class of quantum simulators (as the ones which we previously cited) are “Hamiltonian-based.” In this setting, the experimenter is supposed to be able to turn on and turn off Hamiltonians from a given set. Another class of quantum simulators are quantum cellular automata (QCA) (see Refs. [19–25] and the recent reviews [26,27]) which consist of a translational invariant network of local quantum gates implementing the discrete-time evolution of a lattice of quantum systems, each one interacting only with a finite number of neighbors. QCAs and in particular quantum walks (QWs) [28], which can be thought of as the one particle sectors of QCAs, have been considered as a simulation tool for relativistic quantum fields [29–35] and as discrete approaches for studying the foundations of quantum field theory [34,36–39].

Once a simulation framework has been chosen, one needs some tools to assess the quality of the simulation and quantify how close the evolution of the discrete model and that of the target system are. This is usually achieved by applying the Lie-Trotter-Kato product formula [40] as shown in Ref. [2] for a quantum system whose Hamiltonian is the sum of local interactions, i.e., $H = \sum_{i=1}^k H_i$. Then, the discrete time-step evolution $(e^{iH_1\tau} \dots e^{iH_k\tau})^{t/\tau}$ [41] approaches the target evolution e^{iHt} as $\tau \rightarrow 0$ [44]. Typically, if a fixed error threshold must not be exceeded, the larger t is, the smaller τ has to be: long time evolutions demand quantum simulators, which evolve over very short time steps. For finite dimensional systems, a detailed account of the errors for quantum simulations based on product formulas can be given [46,47].

What happens now if we consider the limit $t \rightarrow \infty$? This is the situation we encounter in scattering processes [48,49] in which we study the evolution of wave packets whose evolution is asymptotically free in the far past and in the far future. The scattering operator (or S matrix) is a key source of information about a physical system, and hence the importance of understanding it in quantum simulators with a discrete time evolution. Since an S matrix can be defined only for infinite dimensional systems, the methods employed for finite dimensional systems are no longer of use. Moreover, we cannot even generally claim that the scattering operator of a continuous-time theory is the limit of the scattering operator of a Trotterized model. This would be true if the two limits $\tau \rightarrow 0$ (for the convergence of the Lie-Trotter-Kato formula) and $t \rightarrow \infty$ (inherent in the

definition of the S matrix) commuted. From the Moore-Osgood theorem, a sufficient condition for the exchange of two limits is the uniform convergence of one of the two. Unfortunately, the limit of the Lie-Trotter-Kato formula is generally only locally uniform in t [50].

One could bypass this technical issue by considering a finite dimensional simulation that runs for a sufficiently large time T such that the scattering process takes place. This is a standard procedure and it is the one implemented by Ref. [7], which addresses the problem of simulating scattering amplitudes in quantum field theory. This approach has the technical advantage that the problem can be analyzed in a more manageable finite-dimensional framework and the mathematical tools of, for example, Ref. [51] can be applied in order to assess the error. On the other hand, this procedure is not optimized for scattering processes since it requires that any process, not only the scattering ones, is simulated within the same error threshold. We may expect that, if we focus on scattering amplitudes (and maybe only a subset of them), then the time step τ (required to obtain the same fidelity) could be smaller. A parallel reasoning has been made in Ref. [52], where the error introduced by the Lie-Trotter-Kato formula has been evaluated for localized observables.

Therefore, we are asking the following question: how small does τ have to be such that the scattering amplitudes of the discrete-time simulation reliably recover the scattering amplitudes of the continuous model?

In this Letter we make the first fundamental steps to answering such a question. We develop the theoretical tools needed to define and compute the scattering operator for a quantum system whose time evolution is discrete. We will show how to adapt some of the tools of standard continuous time scattering theory to the discrete time case. In particular, we have two approaches to the perturbative expansion for the S matrix: the first one is analogous to the expansion of the Lippmann-Schwinger equation, the second one to the Dyson series of perturbative quantum field theory. Our analysis will show that time discreteness can introduce a richer diversity of scattering phenomena. This is an analogous of the Umklapp scattering in solid state physics and it is due to the fact that, for discrete time evolution, the quasienergy is conserved modulo a constant.

We then discuss the comparison between the scattering amplitudes of a continuous-time theory and the ones of a corresponding discrete-time one. For systems with bounded energy, we prove and quantify the convergence of the discrete-time scattering amplitudes to the continuous time one as the discretization step τ goes to 0.

Finally, we apply the theoretical analysis to a one-dimensional discrete model for which the two-particle dynamics is analytically known.

General scattering theory for discrete-time dynamics.— Let us assume that a single time-step evolution is described by the unitary operator $U \in \mathcal{B}(\mathcal{H})$ which may describe

many particles in interaction or one particle with a potential. We denote with $U_0 \in \mathcal{B}(\mathcal{H})$ the corresponding free evolution, i.e., the evolution of our quantum system when the interaction (or the potential) is neglected. As usual, we assume that U_0 is “easy,” in the sense that it can be fully diagonalized (e.g., $U_0 = e^{-iH_0}$ with $H_0 = (\hbar^2/2m)\nabla^2$, the Hamiltonian of a nonrelativistic free particle). In this Letter we will consider elastic scattering processes, the generalization to multichannel scattering being left for future works. The main issue in a theory of scattering is to give a precise meaning to the statement “ $U^n|\psi\rangle$ looks asymptotically free as $n \rightarrow -\infty$.” For that statement to be true, there must be a state $|\psi\rangle_{\text{in}} \in \mathcal{H}$ such that $\lim_{n \rightarrow -\infty} \|U_0^n|\psi\rangle_{\text{in}} - U^n|\psi\rangle_{\text{in}}\| = 0$. An analogous statement can be made for the future asymptotic regime ($n \rightarrow +\infty$). Therefore, one requires that the wave operators Ω_{\pm}

$$\Omega_{\pm} := s\text{-}\lim_{n \rightarrow \mp\infty} U^{\pm n} U_0^n P_{\text{ac}}(U_0), \quad (1)$$

exist [48] [s-lim is the limit in the strong operator topology, and $P_{\text{ac}}(U_0)$ is the projector on the subspace of absolute continuity of U_0]. As is the case in most applications, we will assume that U_0 has only an absolute continuous spectrum and has a generalized eigenvector expansion of the kind

$$U_0 = \int_B e^{-i\omega(k)} |k\rangle \langle k| dk, \quad (2)$$

where $B \subseteq \mathbb{R}^n$, $\omega(k)$ is smooth, and we employed the Dirac notation for generalised eigenvectors [53]. For example, if U_0 describes the evolution of a free particle, then k denotes the momentum and $B = \mathbb{R}^3$. On the other hand, if the particle evolves on a discrete lattice then $B \subseteq \mathbb{R}^n$ is the first Brillouin zone and k is the quasimomentum.

The existence of the wave operators is a nontrivial and central problem in scattering theory. Reference [54] proves a nice generalization of the Kato-Rosenblum theorem for unitaries which states that, if $U - U_0$ is a trace-class operator, then Ω_{\pm} exist and $\text{Ran}(\Omega_+) = \text{Ran}(\Omega_-) = \text{Ran}[P_{\text{ac}}(U)]$. If Ω_{\pm} exist, it is easy to see that they are isometric ($\Omega_{\pm}^{\dagger} \Omega_{\pm} = I$) and obey the intertwining relation

$$U \Omega_{\pm} = \Omega_{\pm} U_0. \quad (3)$$

Moreover, if Ω_{\pm} have the same range, $\text{Ran}(\Omega_+) = \text{Ran}(\Omega_-)$, the scattering operator (or S matrix)

$$S := \Omega_-^{\dagger} \Omega_+, \quad (4)$$

is a unitary operator. The S matrix is the operator that relates *in* and *out* asymptotes, i.e., incoming and outgoing particles, and it is the main object of scattering theory.

A straightforward consequence of Eq. (3) is the following commutation relation:

$$[S, U_0] = 0. \quad (5)$$

Despite its simplicity, Eq. (5) has important consequences. The analogous equation for a continuous time dynamics would have been $[S, e^{-iH_0 t}] = 0$ for any $t \in \mathbb{R}$, which implies $[S, H_0] = 0$: namely, scattering processes conserve the energy. However, there exists more than one exponential representation of a unitary operator; for example, we may have $U_0 = e^{-iH_0}$ with $H_0 = \int_{\mathbb{R}} p^2 dE_p$ or $U_0 = e^{-i\tilde{H}_0}$ with $\tilde{H}_0 = \int_{\mathbb{R}} (p^2 \bmod 2\pi) dE_p$: the energy eigenstates whose corresponding eigenvalues differ by 2π are identified. Therefore, from Eq. (5) we may only infer that (quasi-)energy is conserved “modulo 2π ” (in the characteristic units of the discretized model). This feature is also present in quantum systems with a time-period driving [55]. Such a periodicity in the energy conservation is responsible for a richer scattering phenomenology in discrete time models. This effect bears analogies with the Umklapp scattering in solid state physics which is caused by the periodicity in momentum space due to space discretization. In the following we will further discuss this feature with the help of an explicit example.

Perturbative methods: The Lippmann-Schwinger equation.—Once we know that the scattering operator of our dynamical model is well defined, we need techniques that allow us to compute the probability amplitude of scattering processes. In the continuous-time framework, these tools can be provided by an iterative solution of the Lippmann-Schwinger equation within time-independent perturbation theory. We now show the analogous of this perturbative method for the discrete-time case.

As in the continuous case, the starting point is the assumption that the expression $\Omega_{\pm}|k\rangle$, suitably interpreted, is well defined [56]. Then, we can show [57] that the improper matrix elements of the scattering matrix are given by the following equation:

$$\begin{aligned} \langle k'|S - I|k\rangle &= \lim_{\epsilon \rightarrow 0^+} 2\pi\delta_{2\pi}[\omega(k') - \omega(k)] \\ &\quad \times \langle k'|T(e^{-i\omega(k)+\epsilon})|k\rangle, \\ T(z) &:= W + WG(z)U_0W, \quad W := U_0^\dagger U - I, \end{aligned} \quad (6)$$

where $G(z) = (zI - U)^{-1}$ is the resolvent of U and $\delta_{2\pi}(x)$ denotes the Dirac comb with period equal to 2π . The operator $G(z)$ obeys the Lippmann-Schwinger equation $G(z) = G_0(z) + G_0(z)(U - U_0)G(z)$ [where $G_0(z) := (zI - U_0)^{-1}$], which yields to the following Lippmann-Schwinger equation for $T(z)$:

$$T(z) = W + WG_0(z)U_0T(z), \quad (7)$$

whose solution can be formally given in terms of the following Born series

$$T(z) = \sum_{n=0}^{\infty} (WG_0(z)U_0)^n W. \quad (8)$$

By substituting Eq. (8) in Eq. (6) we obtain a series expansion for the matrix elements of S

$$\begin{aligned} \langle k'|S - I|k\rangle &= 2\pi\delta_{2\pi}[\omega(k') - \omega(k)] \cdot \lim_{\epsilon \rightarrow 0^+} [\langle k'|W|k\rangle \\ &\quad + \langle k'|WG_0(e^{-i\omega(k)+\epsilon})U_0W|k\rangle + \dots]. \end{aligned} \quad (9)$$

The convergence of the Born series depends on the existence of the inverse of the operator $I - (U_0^\dagger U - I)G_0(z)U_0$ and therefore on the spectral radius of $(U_0^\dagger U - I)G_0(z)$. Let us consider the simplest case in which $U = U_0V_\chi$ is the product of a free evolution U_0 and $V_\chi := \sum_x e^{-i\chi f(x)}|x\rangle\langle x|$ with $f(x) \neq 0$ only on a finite set. Then $(U_0^\dagger U - I)$ is of finite rank and the convergence of the Born series can be easily established. In particular, it always converges for sufficiently small χ .

Discrete-time scattering vs continuous-time scattering.—The formalism of the previous section allows us to address comparison between the scattering amplitudes of a continuous-time theory described by a Hamiltonian $H := H_0 + V$, with a bounded potential $|V| < +\infty$, and the scattering amplitudes of the discretized theory $U := e^{-iH_0\tau}e^{-iV\tau}$ (τ is the size of the temporal step).

Let us remind that, if we denote with S^c the scattering operator of the continuous theory, we have $\langle k'|S^c - I|k\rangle = -2\pi i\delta(\omega_{k'} - \omega_k)\langle k'|T^{(c)}(\omega_k + i\epsilon)|k\rangle$, where $T^{(c)}$ obeys $T^{(c)}(z) = V + VG_0^{(c)}(z)T^{(c)}(z)$ with $G_0^{(c)}(z) := (z - H_0)^{-1}$. On the other hand, $S^{(\tau)}$ will denote the scattering operator of the discrete theory: $\langle k'|S^{(\tau)} - I|k\rangle = -2\pi i\delta_{2\pi/\tau}(\omega_{k'} - \omega_k)\langle k'|T^{(\tau)}(e^{-i(\omega_k + i\epsilon)\tau})|k\rangle$, where $T^{(\tau)}(z) := (i/\tau)T(z)$ and $T(z)$ was defined in Eq. (6). Let us make the following assumptions: (i) the spectrum of H_0 is upper bounded by ω_M ; this condition applies to a lattice theory with a bounded number of particles with $\omega_M := N\omega_{\max}$ where $\omega_{\max} := \max_{k \in \mathbb{B}} \omega_k$ and N is the maximum number of particles. (ii) $|G_0^{(c)}(\omega_k + i\epsilon)V| = \gamma < 1$; this technical assumption guarantees the existence of $(I - G_0^{(c)}V)^{-1}$ and convergence of the Born series. Then we can prove [57] that

$$\tau \leq \min\left(\frac{\sqrt{2-\gamma}-1}{|V|}, \frac{\pi}{\omega_M}\right) \Rightarrow T^{(\tau)} - T^{(c)} = \tau R(\tau), \quad (10)$$

where the operator valued function $R(\tau)$ is holomorphic in τ and bounded. Equation (10) rigorously proves the convergence $S^{(\tau)} \xrightarrow{\tau \rightarrow 0} S^{(c)}$. At the leading order in τ we have

$$\begin{aligned} & \langle k' | S^{(\tau)} - S^{(c)} | k \rangle \\ &= -2\pi\delta(\omega_{k'} - \omega_k) \cdot \tau \langle k' | T^{(c)}(\omega_k + i\epsilon) V | k \rangle + O(\tau^2). \end{aligned} \quad (11)$$

By further expanding $T^{(c)}(\omega_k + i\epsilon)$ in Eq. (11) as a function of V we obtain $\langle k' | S^{(\tau)} - S^{(c)} | k \rangle = -2\pi\tau\delta(\omega_{k'} - \omega_k) \langle k' | V^2 | k \rangle + O(\tau|V|^3) + O(\tau^2)$ which shows that the first deviation introduced by the discretization are quadratic in the potential.

The bound for τ in Eq. (10) quantifies the intuition that a larger energy band and a stronger potential demands smaller time steps if we want that the scattering amplitudes of the discrete model and the ones of the continuous model are close to each other. In particular, the condition $\omega_M\tau \leq 2\pi$, guarantees that $\delta_{2\pi/\tau}(\omega_{k'} - \omega_k) = \delta(\omega_{k'} - \omega_k)$ and scattering processes between states with different energy values are suppressed. This condition is necessary for the convergence $S^{(\tau)} \xrightarrow{\tau \rightarrow 0} S^{(c)}$. If the spectrum of the energy is not bounded, i.e., $\omega_M = +\infty$ then the suppression of scattering processes at different energy is possible only if $\langle k' | T^{(\tau)}(e^{-i(\omega_k + i\epsilon)\tau}) | k \rangle \rightarrow 0$ as $\tau \rightarrow 0$ for any k, k' such that $\omega_k = \omega_{k'} + 2\pi n/\tau$, $n \in \mathbb{Z}$. This depends on the model at hand and such an analysis is beyond the scope of the present Letter. However, one has that at the leading order $T^{(\tau)}(e^{-i(\omega_k + i\epsilon)\tau}) = V + O(V^2)$ the condition is satisfied provided that the Fourier transform of the potential $\hat{V}(k, k')$ decays sufficiently rapidly as $|k - k'| \rightarrow +\infty$. For example, in the limit case of $V(x) = \delta(x)$ this condition cannot be satisfied and the convergence $S^{(\tau)} \xrightarrow{\tau \rightarrow 0} S^{(c)}$ is not achieved.

Perturbative methods: Interaction picture and Dyson's formula.—A typical situation is the one in which the single-step unitary evolution has the form

$$\begin{aligned} U &:= U_0 U_{\text{int}} = e^{-iH_0} e^{-i\chi H_{\text{int}}}, \\ U_0 &:= e^{-iH_0}, \quad U_{\text{int}} := e^{-i\chi H_{\text{int}}}, \end{aligned} \quad (12)$$

where H_0 denotes a free evolution Hamiltonian, H_{int} is an interaction Hamiltonian and χ is a coupling constant (both H_0 and H_{int} are assumed to be time independent). This is the situation one encounters (up to a scale factor) when simulating a Hamiltonian of the kind $H_0 + \lambda H_{\text{int}}$ by alternating one step of a free evolution and one step of interaction. In this case, it is convenient to represent the dynamics in the interaction picture as follows:

$$\begin{aligned} |\psi(t)\rangle_I &:= U_0^{\dagger t} |\psi(t)\rangle_S, \quad O_I(t) := U_0^{\dagger t} O_S U_0^t, \\ |\psi(t+1)\rangle_S &= U |\psi(t)\rangle_S, \quad O_S := O_S(t) = O_S(0), \end{aligned} \quad (13)$$

where $|\psi(t)\rangle$ is a generic state, O is a generic operator, and the subscripts S and I denote the Schrödinger and

interaction picture, respectively. From Eq. (13) the time evolution in the interaction picture is easily derived:

$$\begin{aligned} |\psi(t+1)\rangle_I &= U_I(t) |\psi(t)\rangle_I, \\ U_I(t) &:= U_0^{\dagger t} U_{\text{int}} U_0^t = U_0^{\dagger t} e^{-i\chi H_{\text{int}}} U_0^t = e^{-i\chi H_I(t)}, \end{aligned} \quad (14)$$

where we used Eq. (12) and $H_I(t) := U_0^{\dagger t} H_{\text{int}} U_0^t$ is the interaction Hamiltonian in the interaction picture. If we solve Eq. (14) for an arbitrary time we obtain Dyson's formula for discrete time dynamics:

$$\begin{aligned} |\psi(t')\rangle_I &= U_I(t', t) |\psi(t)\rangle_I, \\ U_I(t', t) &:= \mathbb{T} \left[\prod_{s=t}^{t'-1} U_I(s) \right] = \mathbb{T} \left[\exp \left(-i\chi \sum_{s=t}^{t'-1} H_I(s) \right) \right], \end{aligned} \quad (15)$$

where \mathbb{T} is the time ordering operator, such that $\mathbb{T}[A(t_1)B(t_2)] = \theta(t_1 - t_2)A(t_1)B(t_2) + \theta(t_2 - t_1)B(t_2)A(t_1)$, $\theta(x)$ denoting the Heaviside function. If it exists, the scattering operator in the interaction picture is given by

$$S = \text{s-lim}_{t \rightarrow +\infty} U_I(t, -t). \quad (16)$$

Equation (15) allows us to compute matrix elements of the scattering operator as a formal power series in the coupling constant χ . For a theory on a lattice with local interactions $H_{\text{int}} := \sum_x H_{\text{int}}(x)$ we have

$$\langle \psi | S | \phi \rangle = \sum_{n=0}^{+\infty} \frac{(-i\chi)^n}{n!} \sum_{t_j, x_j} \langle \psi | \mathbb{T} \left[\prod_{j=1}^n H_I(t_j, x_j) \right] | \phi \rangle, \quad (17)$$

We observe that each term of the expansion conserves the energy modulo 2π and, if the interaction is local, the total momentum is conserved modulo 2π . In many cases, $H_{\text{int}}(x)$ is a polynomial in the field operators and, from Eq. (17), we need to compute time-ordered products of field operators. The evaluation of the terms appearing in the perturbation expansion of the S matrix can be performed by applying Wick's theorem and can diagrammatically be represented in terms of Feynman diagrams.

The Thirring cellular automaton.—We will now apply the techniques of the previous paragraphs to a one-dimensional Fermionic cellular automaton with a four-Fermion on-site interaction, called Thirring quantum cellular automaton [58]. A two-component fermionic field $\psi := (\psi_{\uparrow}, \psi_{\downarrow})^T$ is defined at every lattice site $x \in \mathbb{Z}$ (see Fig. 1) and its single step evolution is given by the unitary operator:

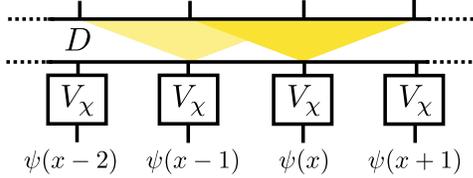


FIG. 1. Thirring QCA unitary step. Each site of the lattice corresponds to a two-component fermionic field $\psi(x)$. The interaction V_χ is completely local while the free evolution D involves the nearest neighbors.

$$\begin{aligned}
 U &:= DV_\chi, & V_\chi &:= e^{i\chi} \sum_{x \in \mathbb{Z}} \psi_\uparrow^\dagger(x) \psi_\uparrow(x) \psi_\downarrow^\dagger(x) \psi_\downarrow(x), \\
 D^\dagger \psi_\uparrow(x, t-1) D &= \nu \psi_\uparrow(x-1, t) - i\mu \psi_\downarrow(x, t), \\
 D^\dagger \psi_\downarrow(x, t-1) D &= \nu \psi_\downarrow(x+1, t) - i\mu \psi_\uparrow(x, t), \\
 \nu, \mu &\in [0, 1], & \nu^2 + \mu^2 &= 1, & \chi &\in (-\pi, \pi]. \quad (18)
 \end{aligned}$$

The vacuum state of the model and a basis for the Fock space are defined as follows:

$$\begin{aligned}
 |\Omega\rangle \text{ s.t. } \psi_\uparrow(x)|\Omega\rangle &= \psi_\downarrow(x)|\Omega\rangle = 0 \quad \forall x \in \mathbb{Z}, \\
 |a_1, x_1; \dots; a_n, x_n\rangle &:= \psi_{a_1}^\dagger(x_1) \dots \psi_{a_n}^\dagger(x_n) |\Omega\rangle. \quad (19)
 \end{aligned}$$

The unitary operator D describes the free evolution (occurring in discrete time steps) of massive Dirac fermions on a one-dimensional lattice and can be diagonalized as

$$\begin{aligned}
 D &= e^{-iH_D}, & H_D &:= \int_{-\pi}^{\pi} dk \sum_{s=\pm} s \omega(k) \psi_s^\dagger(k) \psi_s(k) \\
 \psi_s(k) &:= \sum_{x \in \mathbb{Z}} \frac{e^{-ikx} [\mu \psi_\uparrow(x) + g_s(k) \psi_\downarrow(x)]}{(2\pi)^{1/2} |N_s(k)|}, \quad (20)
 \end{aligned}$$

where $\omega(k) := \arccos(\nu \cos k)$, $|N_s(k)|^2 = \mu^2 + |g_s(k)|^2$ and $g_s(k) = s \sin \omega(k) + \nu \sin k$. The nonlinear evolution V_χ is characterized by the four-fermion interaction of the Thirring and the Hubbard models [59–62]. We notice that, as a consequence of definition (19), the Hamiltonian H_D is not positive definite [hence the states of Eq. (19) are sometimes referred to as *pseudoparticle* states]. As the full evolution U preserves the number of particles, it is convenient to study the dynamics in this representation.

The two particle sector of this quantum cellular automaton can be analytically solved [58] and it is an ideal test for the perturbative methods previously introduced. We can show [57] that the matrix elements of S reads as follows:

$$\begin{aligned}
 \langle k'_1, s'_1; k'_2, s'_2 | S - I | k_1, s_1; k_2, s_2 \rangle \\
 = \delta_{4\pi}(2p - 2p') \delta_{2\pi}(\omega - \omega') \sum_{n=0}^{\infty} (e^{i\chi} - 1)^{n+1} \gamma_n, \quad (21)
 \end{aligned}$$

where we defined $\omega := s_1 \omega(k_1) + s_2 \omega(k_2)$, $\omega' := s'_1 \omega(k'_1) + s'_2 \omega(k'_2)$ and γ_n are suitable coefficients which depend on k_i, s_i, k'_i, s'_i . From Eq. (21) it is clear that processes in which there is a transition between different values of the quasienergy are allowed. The scattering processes for the Thirring automaton can also be perturbatively evaluated by applying Eq. (17). The terms of the perturbative expansion can be labeled by Feynman diagrams. We have, e.g.,

$$\begin{aligned}
 \langle (k'_1 + \pi), -; (k'_2 + \pi), - | S - I | k_1, +; k_2, + \rangle &= \\
 = \chi + \chi^2 + \dots &= \\
 = \delta(k_1 - k'_1) \delta(k_2 - k'_2) (i h_{k_1, k_2} \chi + 2 h_{k_1, k_2}^2 \chi^2 + o(\chi^2)).
 \end{aligned}$$

where h_{k_1, k_2} are suitable coefficients. We notice the following technical detail which has no counterpart in the continuous case: the iterative solution of the Lippmann-Schwinger equation leads to a power series in the variable $\lambda = e^{i\chi} - 1$, while the Dyson series is an expansion in the variable χ . By expanding λ in powers of χ one can check that the two approaches agree.

Discussion.—In this work we analyzed scattering processes for quantum systems which evolve in discrete time steps. We showed how to adapt some of the theoretical tools of continuous-time systems to the discrete case. Both the expansion of the Lippmann-Schwinger equation and the Dyson series maintain a formal analogy with their continuous counterparts. However, some intuitions must be modified, most notably the notion of energy is replaced by quasienergy: just like momentum in a lattice is defined only up to a reciprocal lattice vector, if time in discrete energy is defined only modulo $2\pi/\tau$ (τ is the time step). This feature is also characteristic of periodically driven quantum systems. The periodicity in energy conservation allows for a wider multiplicity of scattering processes as we have seen in the case of the Thirring automaton.

We also discussed how the scattering amplitudes of the Trotterized model can recover the ones of a continuous-time theory. A rather exhaustive assessment, conveyed by Eqs. (10) and (11), can be given if the free Hamiltonian is bounded, as in a lattice theory with bounded numbers of particles. In this case, if the time step τ is sufficiently small [see Eq. (10)], the scattering between different values of energy are suppressed and the discrete-time scattering amplitudes equal the amplitudes of the continuous model plus an analytic function of τ that vanishes in the limit $\tau \rightarrow 0$. In the case of the unbounded spectrum, the suppression of scattering between different energy states cannot be established from the outset but it requires a deeper examination of the dynamics, a necessary condition being a rapid decay of the Fourier transform of the potential.

The application of the present theoretical framework to the simulation of scattering in a relativistic quantum field

theory raises technical issues, mainly because these models are only defined via a renormalized (asymptotic) perturbative series of the scattering amplitudes. The existing approaches (as the one of Ref. [7]) first consider the simulation (for a finite time T) of a continuous-time lattice Hamiltonian dynamics, then extrapolate a continuum limit by considering smaller and smaller lattice spacings. Following the ideas presented in the present Letter, one could (i) compare the scattering operator of the continuous time lattice theory and the scattering operator of the discrete time theory, and then (ii) extrapolate a (renormalized) continuous limit.

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