

Time-Dependent Wave-Packet Approach to Reactions for Quantum Computation

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We describe a method for obtaining the scattering matrix for nuclear or chemical reactions on a finite lattice. Aside from the preparation of the initial and final states as wave packets, the only other operation required is unitary time evolution, making this approach ideal for simulations on quantum hardware. The central quantity is a time-dependent overlap between incoming and outgoing wave packets whose Fourier transform corresponds to the scattering matrix at fixed energy, from which one can calculate elastic and inelastic cross sections for reactions involving two interacting clusters. Working in Cartesian coordinates enables an efficient encoding of the problem on quantum hardware via the first quantization mapping, with favorable qubit scaling for describing asymptotic scattering states. Within this framework, we describe a quantum algorithm for probing the scattering amplitude through different angles, including the forward direction, which provides access to the total cross section via the optical theorem. We demonstrate our methods through a series of numerical examples, for both elastic and inelastic processes, comparing against exact calculations. The techniques we describe can more readily be extended to a large number of constituent particles than other existing approaches, once fault-tolerant quantum hardware becomes available.

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Quantum scattering theory is governed by the S matrix, which encodes the transition amplitude between asymptotic states [1]. The S matrix is sufficiently general to describe complex reaction processes, including the breakup of a composite system into many possible final-state particles/channels. Nuclei composed of many individual nucleons have been successfully described by discretization to a finite lattice [2]. At low energies with relatively few open channels, it is possible to extract scattering phase shifts from a lattice whose spatial extent is large enough that the scattering wave function achieves its asymptotic form [3–5]. The size of the many-body basis, however, grows rapidly as more particles are introduced, especially for particles carrying spin, isospin, or other quantum numbers. Without additional simplifying assumptions and/or phenomenological parameters (e.g., R -matrix theory [6–12]), the problem quickly becomes intractable on classical computers. Fortunately, such systems can be efficiently encoded on a quantum computer in the first quantization mapping [13–17].

Several algorithms have been proposed to calculate elastic scattering phase shifts on a quantum computer [18–21]. To reliably extract cross sections with such

methods, one must compute the phase shift in partial waves up to $\ell_{\max} \approx kR_0$, where k is the scattering momentum and R_0 is the range of the potential. Moreover, these approaches are not straightforward to generalize to describe reactions with different initial- and final-state particles (i.e., capture or breakup reactions) or scattering between composite systems with internal structure that allows for inelastic transitions.

In this Letter, we describe a method—based on the time-dependent scattering formalism of Tannor and Weeks [22]—for computing total and differential scattering cross sections using wave packets localized within a discrete lattice volume. Time-dependent wave-packet methods have long been employed in classical calculations of chemical reaction dynamics (see, e.g., Refs. [23–25] and references therein). As the wave packets have a finite region of support, they can be propagated to asymptotic separation while remaining localized within the computational volume. Each wave packet contains a mixture of different momentum eigenstates; as a result, a single simulation provides information about the reaction process across a range of scattering energies. Via Fourier transform, we can isolate particular energy components of the S matrix, from which the desired cross sections can be readily obtained.

Our reaction formalism is directly compatible with a first-quantized, lattice-based description of the scattering constituents on quantum hardware: To each particle, we associate some number of qubits that encode the position of the particle within the spatial (or momentum) lattice as well as any additional quantum numbers (e.g., spin and/or

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isospin). Within this framework, we describe quantum algorithms to obtain total and differential cross sections for $2 \rightarrow 2$ scattering, including inelastic processes where the scattering constituents transition between internal eigenstates. A schematic overview of our formalism is presented in [26].

In the present work, we restrict our attention to short-ranged interactions characteristic of the strong nuclear interaction, but the necessary extension of the S -matrix scattering formalism to include Coulomb interactions exists and will be important to implement so that one can simulate charged-particle reactions.

We assume that the initial state is composed of two systems (i.e., a projectile and a target) with respective masses M_1 , M_2 , both of which in general may be composite. The total system is governed by the Hamiltonian

$$H = H_0 + H_{\text{int}} = T_{\text{CM}} + T_{\text{rel}} + h^{(1)} + h^{(2)} + H_{\text{int}}, \quad (1)$$

where T_{CM} and T_{rel} are kinetic energy operators corresponding, respectively, to the center of mass (CM) of the total system and the relative coordinate $\mathbf{r} = (x, y, z)$ that describes the separation of the two clusters; $h^{(i)}$ is the internal Hamiltonian of cluster i consisting of the relative kinetic energy of the constituent particles and their interparticle (intracluster) interactions. The intercluster interaction H_{int} is assumed to be finite range, so that the interaction vanishes (or is exponentially small) when the relative separation r between the two clusters is sufficiently large. Each cluster's internal degrees of freedom are assumed to occupy an eigenstate $|\psi_{\alpha_i}^{(i)}\rangle$ satisfying $h^{(i)}|\psi_{\alpha_i}^{(i)}\rangle = E_{\alpha_i}^{(i)}|\psi_{\alpha_i}^{(i)}\rangle$, with α_i denoting a set of quantum numbers that completely specifies the state. The system will be prepared in a state with zero CM momentum and relative component described by a propagating Gaussian wave packet,

$$\phi_{\text{rel}}(\mathbf{k}_0, \mathbf{r}) = \frac{e^{-z^2/2\sigma^2}}{\sqrt{\sigma\pi^{1/4}}} \frac{e^{i\mathbf{k}_0 \cdot \mathbf{r}}}{2\pi}, \quad (2)$$

so that the total state of the system can be expressed as

$$|\Phi_{\mathbf{k}_0, \alpha}\rangle \equiv |\psi_{\alpha_1}^{(1)}\rangle |\psi_{\alpha_2}^{(2)}\rangle \phi_{\text{rel}}(\mathbf{k}_0, \mathbf{r}), \quad (3)$$

where $\mathbf{k}_0 = (k_{0,x}, k_{0,y}, k_{0,z})$. Along the $\hat{\mathbf{z}}$ axis, the relative wave packet $\phi_{\text{rel}}(\mathbf{k}_0, \mathbf{r})$ has spatial width σ and propagates with group momentum $k_{0,z}$. Along the transverse directions, $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, the relative wave function occupies momentum eigenstates with respective eigenvalues $k_{0,x}$ and $k_{0,y}$.

The original proposal of Tannor and Weeks [22] is formulated in Jacobi coordinates, reducing the computational cost by eliminating the redundant CM degree of

freedom. In contrast, our approach is based on absolute Cartesian coordinates, which map simply to a first-quantized encoding on quantum hardware. Moreover, in Ref. [22], momentum is imparted to the wave packet only along the direction of propagation. By introducing momentum $k_{0,x}$, $k_{0,y}$ along the transverse directions, we are able to probe scattering through different angles, as demonstrated below.

We are primarily interested in transitions between states of definite relative momentum,

$$|\Psi_{\mathbf{k}, \alpha}\rangle \equiv |\psi_{\alpha_1}^{(1)}\rangle |\psi_{\alpha_2}^{(2)}\rangle \sqrt{\frac{\mu}{k}} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{(2\pi)^{3/2}}, \quad (4)$$

chosen here to be normalized with respect to energy. Such states are eigenstates of the noninteracting Hamiltonian H_0 with eigenvalue $E = k^2/2\mu + E_{\alpha_1}^{(1)} + E_{\alpha_2}^{(2)}$, where $\mu = M_1 M_2 / (M_1 + M_2)$ is the reduced mass of the system. The notion of asymptotic states is made precise by introducing the Møller operators [1]

$$\Omega_{\pm} \equiv \lim_{t \rightarrow \mp\infty} e^{iHt} e^{-iH_0 t}. \quad (5)$$

When the Møller operators act on an eigenstate of the noninteracting Hamiltonian H_0 , the resulting state $|\Psi_{\mathbf{k}, \alpha}^{\pm}\rangle \equiv \Omega_{\pm} |\Psi_{\mathbf{k}, \alpha}\rangle$ is an eigenstate of the fully interacting Hamiltonian H with the same energy eigenvalue. Solutions obtained from the action of Ω_+ (Ω_-) are known as outgoing (incoming) scattering solutions.

Suppose that the final state consists of the same two clusters as the initial state; that is, the masses M_1 , M_2 are conserved. (The kinematic modifications required to relax this assumption are straightforward.) Choosing the Gaussian width σ to be unchanged, we allow the initial and final wave packets to have different plane-wave factors, $\mathbf{k}_0 = (k_{0,x}, k_{0,y}, k_{0,z})$ for the initial state and $\mathbf{k}'_0 = (k'_{0,x}, k'_{0,y}, k'_{0,z})$ for the final state. The internal degrees of freedom of each cluster can transition between eigenstates of $h^{(i)}$, so that the initial and final states are labeled by quantum numbers $\alpha = (\alpha_1, \alpha_2)$ and $\beta = (\beta_1, \beta_2)$, respectively. We define the S matrix to be the transition amplitude between outgoing and incoming scattering solutions

$$\langle \Psi_{\mathbf{k}', \beta}^- | \Psi_{\mathbf{k}, \alpha}^+ \rangle = \delta(E' - E) S_{\beta, \alpha}(E, \theta), \quad (6)$$

where $E = k^2/2\mu + E_{\alpha_1}^{(1)} + E_{\alpha_2}^{(2)}$, $E' = k'^2/2\mu + E_{\beta_1}^{(1)} + E_{\beta_2}^{(2)}$, and $\cos \theta = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$ defines the scattering angle θ .

The free-particle solutions $|\Psi_{\mathbf{k}, \alpha}\rangle$ are plane waves in the relative coordinate $\mathbf{r}$ between the two clusters and thus are not spatially localized. The same is true of the corresponding scattering solutions $|\Psi_{\mathbf{k}, \alpha}^{\pm}\rangle$ —beyond the range of the interaction, they coincide with the free solutions, $\Psi_{\mathbf{k}, \alpha}^{\pm}(\mathbf{r}) \sim \Psi_{\mathbf{k}, \alpha}(\mathbf{r})$ as $r \rightarrow \infty$. As a result, it is computationally

difficult to obtain the S matrix directly from the scattering states $|\Psi_{\mathbf{k},\alpha}^{\pm}\rangle$. Instead, we utilize the fact that the asymptotic scattering state can be obtained via energy projection of the corresponding Møller-evolved wave packet [22,26],

$$|\Psi_{\mathbf{k},\alpha}^{\pm}\rangle = \frac{k_z}{2\pi\mu\eta(k_z)} \sqrt{\frac{\mu}{k}} \int_{-\infty}^{+\infty} dt e^{-iHt} |\Phi_{\mathbf{k}_0,\alpha}^{\pm}\rangle e^{iEt}, \quad (7)$$

where $|\Phi_{\mathbf{k}_0,\alpha}^{\pm}\rangle \equiv \Omega_{\pm} |\Phi_{\mathbf{k}_0,\alpha}\rangle$, and the quantities $\mathbf{k}$, $\mathbf{k}_0$, and E are related by

$$k^2 = k_{0,x}^2 + k_{0,y}^2 + k_z^2 = 2\mu(E - E_{\alpha_1}^{(1)} - E_{\alpha_2}^{(2)}). \quad (8)$$

The normalization factor

$$\eta(k_z) = \frac{\sqrt{\sigma}}{\pi^{1/4}} e^{-(k_z - k_{0,z})^2 \sigma^2 / 2} \quad (9)$$

is the amplitude of the momentum mode k_z within the Gaussian wave packet that governs the relative motion. Using Eq. (7), we can express the S matrix in terms of the Møller-evolved plane-wave states as [22,26]

$$S_{\beta,\alpha}(E, \theta) = \frac{1}{2\pi\eta'(k'_z)\eta(k_z)} \frac{k_z k'_z}{\mu\sqrt{kk'}} \times \int_{-\infty}^{+\infty} dt \langle \Phi_{\mathbf{k}'_0,\beta}^- | e^{-iHt} | \Phi_{\mathbf{k}_0,\alpha}^+ \rangle e^{iEt}, \quad (10)$$

where $\eta'(k'_z)$ is analogous to $\eta(k_z)$ with $k_{z,0} \rightarrow k'_{z,0}$.

The central quantity that can be obtained from quantum computation is the dimensionless overlap function

$$C_{\beta,\alpha}(\mathbf{k}'_0, \mathbf{k}_0; t) \equiv \langle \Phi_{\mathbf{k}'_0,\beta}^- | e^{-iHt} | \Phi_{\mathbf{k}_0,\alpha}^+ \rangle. \quad (11)$$

If the overlap function is sampled at sufficiently many times (set by the momentum/energy resolution of the lattice), the subsequent Fourier transform is trivial to perform classically. Assuming that the wave-packet states $|\Phi_{\mathbf{k}_0,\alpha}\rangle$, $|\Phi_{\mathbf{k}'_0,\beta}\rangle$ can be efficiently prepared on a quantum computer, the only other required operation is unitary time evolution. On quantum hardware, the needed time evolution can be performed either by a product expansion (Trotterization) [32] or via quantum signal processing (qubitization) [33]. Reconstructing the S matrix requires both the real and imaginary parts of the overlap function, obtained from respective Hadamard tests using a single set of particle qubit registers [26]. A Hadamard test requires $\mathcal{O}(\epsilon^{-2})$ measurements, where ϵ is the targeted error. The number of time samples will depend on the system and the simulation box size [26].

The correlation function contains contributions to the S matrix from all incident energies represented within the initial and final wave packets, and as a result the measured signal is large enough to be distinguished from the noise. Because the wave packets are extended plane waves in $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, the contributions to the cross section from all impact parameters are automatically included, further increasing the signal.

The procedure outlined above requires propagation of the initial and final wave packets to infinite times $t \rightarrow \pm\infty$, which is not feasible. However, it suffices to evolve the initial and final wave packets to an asymptotic time t_{∞} , which is chosen to be large enough that the interaction between the wave packets is exponentially suppressed but small enough that they have not yet incurred significant edge effects from the periodic boundary conditions. As such, the $t \rightarrow \pm\infty$ limits appearing in the Møller operators [Eq. (5)] can be replaced by a finite asymptotic time $\pm t_{\infty}$. Similarly, the limits of integration in Eq. (10) can also be replaced by $\pm t_{\infty}$. The appropriate value of t_{∞} depends on the nature of the scattering problem, the wave packets, and the lattice size [26]. In principle, one can choose different asymptotic times $t_{-\infty}$ and $t_{+\infty}$ for Ω_+ and Ω_- and the limits of integration of the overlap function.

As discussed above, our formalism assumes a first-quantized description of the scattering constituents. In this way, the total kinetic energy operator $T = \sum_i T_i$ acts independently on each single-particle Hilbert space and therefore can be efficiently implemented on a quantum computer [17,34]. The tradeoff is that either the initial or final wave packets must be projected onto a state with definite CM momentum, assumed here to be the zero-momentum state. As described further in [26], the required projection can be efficiently performed with either standard quantum phase estimation (see, e.g., Ref. [35]) or the projection algorithm introduced in Ref. [28]. If we were to work directly in relative (or Jacobi) coordinates, as in Ref. [22], then the kinetic energy operator restricted to this subspace will not in general factorize across single-particle Hilbert spaces nor necessarily admit an efficient quantum circuit implementation.

The S matrix obtained from a finite-volume calculation is a volume-dependent quantity—for a fixed interaction, increasing the side length L of the box decreases the proportion of the scattered wave relative to the incoming wave. Nonetheless, it is straightforward to exchange the volume-dependent S matrix for the volume-independent scattering amplitude $f_{\beta,\alpha}(E, \theta)$ [36],

$$S_{\beta,\alpha}(E, \theta) = \delta_{\beta,\alpha} \delta_{\theta} + \frac{2\pi i}{\sqrt{kk'} L^2} f_{\beta,\alpha}(E, \theta), \quad (12)$$

where $\delta_{\theta} = 1$ if $\theta = 0$ and $\delta_{\theta} = 0$ if $\theta \neq 0$. The differential cross section $d\sigma_{\beta,\alpha}/d\Omega$ and total cross section $\sigma_{\beta,\alpha}$ corresponding to specific transitions between internal eigenstates

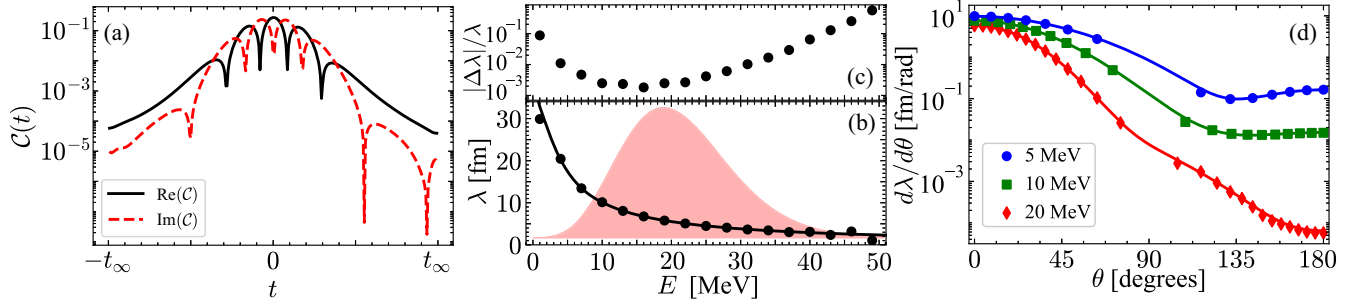


FIG. 1. Elastic two-body scattering in two spatial dimensions by an attractive Gaussian potential [see Eq. (14)]. (a) Overlap function $C(t) \equiv C(\mathbf{k}'_0, \mathbf{k}_0; t)$ for forward scattering, $\mathbf{k}'_0 = \mathbf{k}_0 = (0, k_{0,y})$. Solid black and dashed red lines denote, respectively, the real and imaginary parts of the overlap function. (b) Total cross section λ as a function of energy, obtained from the forward-scattering amplitude via the optical theorem. The red shaded region shows the relative energy profile of the wave packets (arbitrary normalization). (c) Relative error $|\Delta\lambda|/\lambda$ between the wave-packet and variable-phase results. (d) Differential cross section $d\lambda/d\theta$ at three different scattering energies, $E = 5, 10$, and 20 MeV. In panels (b) and (d), solid lines denote the exact numerical result obtained via the variable phase method [27,37] (adapted to two spatial dimensions); data points were obtained via the time-dependent wave-packet formalism.

$\alpha \rightarrow \beta$ can thus be obtained as

$$\frac{d\sigma_{\beta,\alpha}}{d\Omega} = |f_{\beta,\alpha}(E, \theta)|^2, \quad \sigma_{\beta,\alpha} = \int d\Omega \frac{d\sigma_{\beta,\alpha}}{d\Omega}. \quad (13)$$

Numerical examples—We demonstrate our methods with a series of numerical examples performed as classical computations. Due to the complexity of these calculations, we restrict our examples to two spatial dimensions. Scattering theory in two dimensions [29] shares many of the pertinent features of its three-dimensional analog. We consider a system of two nucleons with $M_1 = M_2 = m_N = 938.92$ MeV/ c^2 interacting via the Gaussian potential

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = V_0 U(r) = V_0 \exp(-r^2/2R_0^2), \quad (14)$$

with $V_0 = -10$ MeV and $R_0 = 2.63$ fm. The resulting interaction is a satisfactory model of the strong nuclear force between two nucleons, resulting in a single bound state with energy $E_d = -2.225$ MeV, albeit in two spatial dimensions. Each particle has a Hilbert space corresponding to a 64^2 spatial lattice with lattice constant $a = 1.9$ fm. In the first quantization mapping, this system could be represented by 12 logical qubits per particle. The kinetic energy is treated exactly via Fourier transform; for implementation on quantum hardware, it may be advantageous to instead employ a finite difference approximation. The scattering constituents under consideration have no internal degrees of freedom, and we will hereafter omit the eigenstate labels α, β .

The wave packets were chosen to have spatial width $\sigma = 5.39$ fm. The initial and final wave-packet momenta were chosen to be $\mathbf{k}_0 = (0, k_{0,y})$, $\mathbf{k}'_0 = (k'_{0,x}, k'_{0,y})$ with $|k_{0,y}| = |k'_{0,y}| = 0.644$ fm $^{-1}$. (In two spatial dimensions, we assume that $\hat{\mathbf{y}}$ is the direction along which the wave packet propagates.) To consider scattering through angles

$0^\circ \leq \theta \leq 90^\circ$, we take $k_{0,y} = k'_{0,y}$ and vary the transverse momentum of the final state $k'_{0,x}$ over all allowed lattice momenta. Backscattering ($90^\circ \leq \theta \leq 180^\circ$) is assessed via the same procedure but with $k_{0,y} = -k'_{0,y}$. (In three spatial dimensions, the scattering angle $\cos\theta = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$ can be varied analogously, thus avoiding the cumbersome formulation of Jacobi coordinates.) To prepare the Møller states, the wave packets were evolved to time $t_\infty = 1.08$ MeV $^{-1}$. Further technical details are provided in [26].

Forward scattering corresponds to $k'_{0,x} = 0$. After forming the Møller-evolved wave packets $|\Phi_{\mathbf{k}_0}^+\rangle, |\Phi_{\mathbf{k}'_0}^-\rangle$ one obtains the overlap function shown in Fig. 1(a). Performing the Fourier transform of this overlap function, as in Eq. (10), one can obtain the forward-scattering matrix $S(E, 0)$ at any energy E where the wave packets have significant support. Relating this result to the forward-scattering amplitude $f(E, 0)$ via the two-dimensional analog of Eq. (12) (see Ref. [26]), one can obtain the total cross section from the two-dimensional optical theorem [29], $\lambda = \sqrt{8\pi}/k \text{Im} f(E, 0)$.

The considered energy need not correspond to the energy of one of the lattice eigenstates; although the lattice calculation consists of a discrete basis of particular eigenmodes, the resulting overlap function smoothly interpolates between them. This property is evident in Fig. 1(b), where the total cross section is computed at evenly spaced scattering energies $E = 1, 4, \dots, 49$ MeV, which do not correspond to lattice eigenenergies. As shown in the same figure, the chosen wave packets have appreciable support for scattering energies $5 \lesssim E \lesssim 40$ MeV. Within this region, the relative error on the cross section is typically much less than 1%, as shown in Fig. 1(c).

Figure 1(d) shows the angular differential cross section $d\lambda/d\theta$ at three different scattering energies, $E = 5, 10$, and 20 MeV. As the transverse momentum $k'_{0,x}$ must correspond to a lattice eigenstate, only a specific finite set of scattering

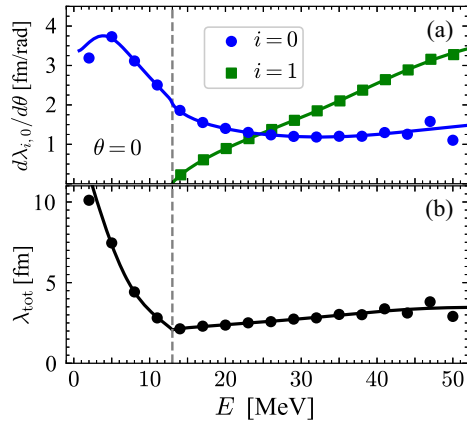


FIG. 2. Two-channel scattering cross sections: (a) Elastic (blue) and inelastic (green) differential cross sections evaluated in the forward limit $\theta = 0$. (b) Total (elastic + inelastic) integrated cross section λ_{tot} obtained via the optical theorem. Solid lines were calculated via the variable-phase method; points correspond to the time-dependent wave-packet formalism. Vertical dashed line denotes the excited state threshold energy, $\Delta = 13$ MeV.

angles can be probed at a given energy, with higher scattering energies admitting more possible angles. The agreement between the wave-packet solution and that obtained by numerical integration in partial waves is generally quite good, even when $\theta \approx \pi$ and the scattering is very weak. Close to $\theta = \pi/2$, the scattering is dominated by momentum modes $k'_{0,x}$ along the transverse direction; in such cases, the projected final-state momentum k'_y is very close to zero and not well represented by the wave packet, leading to comparatively large errors in the cross section.

Existing quantum algorithms for elastic nuclear scattering [18–21] allow one to calculate the partial-wave phase shifts. Depending on the nature of the interaction, constructing the corresponding cross sections could potentially require summation over many partial waves. In the case of a noncentral potential, such as the nuclear tensor interaction, the partial-wave phase shifts can only be obtained by solving a system of coupled equations. Our approach is completely agnostic to the nature of the interaction, as long as it is short ranged. Though for convenience we consider here a central potential, our framework operates identically if the interaction permits the exchange of angular momentum (or other quantum numbers such as spin and isospin) between projectile and target.

Inelastic scattering—To demonstrate the generality of our formalism, we extend the previous example to a two-channel scattering problem with Hamiltonian

$$H = \begin{pmatrix} T + V_0 U(r) & \bar{V}_0 U(r) \\ \bar{V}_0 U(r) & T + \Delta + 2V_0 U(r) \end{pmatrix}, \quad (15)$$

with $U(r)$ as in Eq. (14), and $V_0 = 10$ MeV, $\bar{V}_0 = 14.24$ MeV, and $\Delta = 13$ MeV, chosen such that the system does not have any Feshbach resonances. Let us

label the zero-threshold channel by the quantum number $\alpha = 0$ and the finite-threshold ($\Delta > 0$) channel by $\alpha = 1$. We otherwise adopt identical lattice and wave-packet parameters to those employed in the previous example.

Preparing both the initial and final wave packets in the zero-threshold channel, we obtain the elastic scattering matrix $S_{0,0}(E, \theta)$ and, correspondingly, the elastic differential cross section $d\lambda_{0,0}/d\theta$. Likewise, preparing the initial wave packet in the zero-threshold channel and the final wave packet in the Δ -threshold channel, we obtain the inelastic scattering matrix $S_{1,0}(E, \theta)$ and the inelastic differential cross section $d\lambda_{1,0}/d\theta$. As before, we can probe scattering through different angles by imparting transverse momentum to the final-state wave packets.

Figure 2(a) shows the elastic and inelastic differential cross sections evaluated in the forward limit. As expected, the inelastic cross section vanishes at the threshold energy $\Delta = 13$ MeV. Figure 2(b) shows the total integrated cross section $\lambda_{\text{tot}} = \lambda_{0,0} + \lambda_{1,0}$ obtained from the forward-scattering amplitude $f_{0,0}(E, 0)$ via the optical theorem. As in the previous example, the wave-packet formalism performs very well at energies where the wave packets have appreciable support. [The energy profile employed here is the same as that shown in Fig. 1(b).]

Summary—In this Letter, we describe a time-dependent wave-packet approach to scattering that is ideal for quantum computation in the first quantization mapping. So far, we have restricted our attention to elastic and inelastic scattering of two particles interacting via a short-ranged potential. The approach, however, is general—both the target and the projectile can be composite systems, opening the way for simulation of nuclear and chemical reactions. A detailed error analysis of our formalism is provided in Supplemental Material [26].

The use of wave packets localized to a finite lattice provides scattering information across the entire range of energies where the wave packets have appreciable support. Naturally, the wave packets and the lattice are chosen so that the two clusters can be brought to asymptotic separation without incurring edge effects. The most straightforward means of simulating scattering at lower energies is therefore to increase the spatial extent of the lattice.

Interplay between the wave packets and the lattice also determines the time over which the system can be evolved and over which the central quantity—the overlap function—can be probed. For the relatively fast reactions considered here, the overlap function damps exponentially at long times. For scattering involving resonances or compound states, the overlap function is expected to exhibit long-lived behavior, which can be resolved by employing a lattice with a larger spatial extent. In first quantization, the side length L of a cubic lattice is doubled by introducing one additional qubit per particle per spatial dimension.

In realistic calculations involving identical particles, the scattering constituents must have the proper exchange

symmetry (i.e., symmetric exchange for bosons, antisymmetric for fermions), which is not guaranteed *a priori* of many-body states in first quantization. Fully antisymmetric states can be prepared using one of several antisymmetrization algorithms [14,16,38], including one specialized for antisymmetrizing the constituent particles of a target and projectile that are spatially separated [30].

Elastic/inelastic cross sections can then be calculated by preparing the outgoing products into properly antisymmetrized ground/excited states. While our method targets a specific final state, it naturally accounts for scattering into all energetically open channels. Extending this framework to treat reactions with more than two final-state clusters will require significant modification; the final-state kinematics are less constrained than the two-cluster case, allowing for different momentum-sharing between the outgoing clusters. More straightforward variations of the method outlined in this work will allow for the simulation of charged-particle reactions where the Coulomb force acts between the scattering constituents, as well as the treatment of photo-induced reactions.

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Data availability—The data that support the findings of this article will be made available upon reasonable request.

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