Precise Quantum Simulations with Optical Lattices

Xingze Qiu\(^1\) and Xiaopeng Li\(^1,*\)

\(^1\)State Key Laboratory of Surface Physics, Institute of Nanoelectronics and Quantum Computing, and Department of Physics, Fudan University, Shanghai, 200433, China

(Dated: March 4, 2020)

We present an efficient approach to precisely simulate tight binding models with optical lattices, based on programmable digital-micromirror-device (DMD) techniques. Our approach consists of a subroutine of Wegner-flow enabled precise extraction of a tight-binding model for a given optical potential, and a reverse engineering step of adjusting the potential for a targeting model, for both of which we develop numerical methods to achieve high precision and high efficiency. With renormalization of Wannier functions and high band effects systematically calibrated in our protocol, we show the tight-binding models with programmable onsite energies and tunnelings can be precisely simulated with optical lattices integrated with the DMD techniques. For example, the random hopping Anderson localization model, which is believed to be difficult to reach in optical lattice experiments, can be precisely simulated with our approach. We expect this approach would pave a way towards optical-lattice based precise programmable quantum simulations.

Introduction.— Quantum simulation and quantum computing have been attracting tremendous attention in recent years. Among the rapidly advancing quantum hardwares \([1]\), cold atoms provide a unique quantum simulation platform for their controllability and scalability \([2–5]\). In the last two decades, cold atom based quantum simulations have achieved fantastic progress not only along the line of conceptually novel physics such as artificial gauge fields \([6–8]\), and topological matters \([9]\), but also along the line of simulating computationally difficult problems such as BEC-BCS crossover \([10]\), High-Tc physics \([11–14]\), and non-equilibrium dynamics \([15]\), where its exceptional quantum advantage has been demonstrated.

In quantum simulations aiming for demonstration of novel physical concepts, it is not crucial to precisely calibrate the system. However, in order to use quantum simulations to solve computationally difficult problems, it is required to make the simulation precise—for example in the study of quantum criticality and in solving spin-glass problems, the physical properties of interest are sensitive to Hamiltonian parameters. And in quantum simulations of many-body localization using an incommensurate optical lattice, it has been found that calibration problems cause qualitative disagreement \([16–19]\) with the targeting Aubry-Andre (AA) model \([20, 21]\). This issue also arises generically in using speckle-pattern induced disorder optical potentials to simulate localization physics \([22–33]\), as the onsite energies and tunnelings are not programmable, let alone the simulation precision.

In this work, we consider integration of the recently developed DMD techniques in controlling optical potentials \([12, 34–37]\) to optical lattices, and calibrate the platform towards precise programmable quantum simulations. We develop an efficient numerical optimization method, which can systematically construct an inhomogeneous optical potential to precisely simulate a given tight binding lattice model, i.e., both the onsite energies and the tunnelings are made precisely programmable. For benchmarking, we provide detailed numerical results for AA and Anderson localization (AL) models, where we show our approach has adequate programmability and systematically eliminates calibration errors. Our protocol adds precise programmability to the quantum platform of optical lattice, which is intrinsically demanded for quantum simulations aiming for computationally difficult problems.

Theory setup and numerical method.— For atoms confined in an optical potential, the Hamiltonian description is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_p(x) + V_D(x). \quad (1)$$

Here we have separated the optical potential into a primary part \(V_p(x) = V / 2 \cos(2kx)\) created by standard counter propagating laser beams and an additional potential \(V_D(x)\) created by DMD techniques. The primary part has lattice translation symmetry with the lattice spacing determined by the forming laser wavelength. Hereafter, we use the lattice constant \(a = \pi/k\) as the length unit and the photon recoil energy of the lattice \(E_R = \hbar^2 k^2/2m\) as the energy unit. The added potential \(V_D(x)\) in general has no homogeneity, and with the present technology it is typically much weaker than the primary lattice. A targeting tight-binding Hamiltonian matrix for the continuous system to simulate is referred to as \(\mathcal{H}^*\), which contains onsite energies \(\epsilon_i\) and tunnelings \(J_{i,i'}\), with \(i,i'\) labeling lattice sites determined by the primary optical potential. In the following, we describe our numerical method to reverse engineer \(V_D(x)\) and \(V_p(x)\) that makes the precise
tight-binding model description of $H$ in Eq. (1) our target, $\mathcal{H}^\star$.

Firstly, we describe our method for efficient extraction of a tight-binding model of the continuous Hamiltonian $H$. Without the inhomogeneous potential $V_D(x)$, the precise tight binding model of the system can be efficiently constructed by introducing Bloch modes, because different modes with different lattice momenta are decoupled due to lattice translation symmetry. In the Wannier function basis, the Hamiltonian takes a block diagonalized form with the decoupled blocks corresponding to different bands [38]. In the presence of an inhomogeneous potential $V_D(x)$, the lattice translation symmetry becomes absent, and the Wannier states are coupled within each band and also across different bands. We propose to use Wegner flow [39, 40] to decouple different bands, which then produces a precise tight-binding model. We denote the Hamiltonian matrix in the Wannier function basis as $\mathcal{H}_{m,m'}(l)$, with $m, m'$ labeling different bands running from zero (lowest band) to a high-band cutoff $M$. We propose to use the Wegner function localized centers (or equivalently the lattice sites of the primary lattice). The band decoupling procedure follows a flow equation,

$$\frac{d\mathcal{H}(l)}{dt} = [\eta(l), \mathcal{H}(l)],$$

that generates a continuous unitary transformation $\mathcal{H}(l) = U(l) \mathcal{H}(0) U(l)^\dagger$. Here $\eta(l)$ is an anti-Hermitian matrix, $\frac{dU(l)}{dt} U(l)^\dagger$, which we choose to be $\eta(l) = [G, \mathcal{H}(l)]$, with $G_{m,m'} = \delta_{m,m'} [2\delta_{m,0} - \delta_{m,0} \delta_{m',0}]$. Following the flow from $l = 0$ to $+\infty$, $\mathcal{H}(l)$ converges to a matrix that commutes with $G$ because

$$\text{Tr}[\mathcal{H}(l) - G]^2 \geq 0,$$

$$\frac{d}{dt} \text{Tr}[\mathcal{H}(l) - G]^2 = -2\text{Tr}[\eta(l) \eta(l)] \leq 0.$$

This means the coupling between the $m = 0$ block of the matrix $\mathcal{H}$ and other blocks monotonically converges to 0. The convergence speed in the iteration is inversely proportional to the band gap. This means our approach is applicable as long as the inhomogeneous potential $V_D(x)$ is not too strong to close the band gap. The finite-depth flow equation generates a local unitary that defines a precise tight-binding model as the converged $m = 0$ Hamiltonian block.

Secondly, we develop a numerical optimization method to adjust the potential $V_D(x)$ to minimize the difference between $\mathcal{H}_{\text{eff}}$ and $\mathcal{H}^\star$. We choose a Frobenius-norm based cost function $f = f_0 + \lambda_1 f_1$, where $f_0$ and $f_1$ are Frobenius norms for the difference in the onsite energies and tunnelings, respectively, and a hyper-parameter $\lambda_1$ is introduced to afford extra weight to the tunneling

for better optimization-performance. In our numerics, we parameterize

$$V_D(x) = \sum_{n=0}^{2L-1} \tilde{V}_n \cos \left( \frac{2\pi}{L} kx + \phi_n \right),$$

where $L$ is the number of periods of the primary lattice, and $\tilde{V}_n, \phi_n$ are variational parameters. We start from a random initialization, obtain $\mathcal{H}_{\text{eff}}$ through Wegner flow, and then update the optical potential through a gradient descent method. This procedure is iterated until the cost function is below a threshold of our request.

Furthermore, our method is highly efficient by making use of locality. Considering a system with large system size, instead of performing the Wegner-flow for the full problem which then has a computation complexity of $O(L^3)$, we split the system into small pieces, with an individual length $L_p$. The adjacent pieces have about one third of their length overlapped with each other. We optimize the optical potential to reproduce the precise tight-binding model piece-by-piece, and then glue them together. This is sensible because of the locality in the problem—the onsite energy at one site and the tunnelings between two sites are both determined by their neighboring potential, following the finite-depth Wegner flow. Note that one problem arises that the potential may not be smooth in the overlapping regions, as the obtained potential could be inconsistent in optimizing the two adjacent pieces. To solve this problem, we add $\lambda_2 f_2$ to the cost function, where $f_2$ is the Frobenius norm of the difference of the potential in the overlapping region obtained in the optimization of its belonging two pieces. The piece-by-piece procedure is swept back-and-forth for convergence, analogous to the optimization in the standard density-matrix-renormalization group calculation [41]. In the sweeping process, we find a monotonic decrease in the difference between $\mathcal{H}_{\text{eff}}$ and $\mathcal{H}^\star$ in the whole system, and that the converged optical potential is smooth. The computation complexity scaling is thus reduced to $O(L)$.

**Application to quantum simulation of AA model.**—In the study of quantum localization physics, AA model has been investigated extensively in both theory and experiment [16–19, 27, 42–48]. Its Hamiltonian reads as

$$H^\star_{\text{AA}} = -J_{\text{AA}} \sum_i (c_{i+1}^\dagger c_i + h.c.) + \frac{\Delta_{\text{AA}}}{2} \sum_i \cos(2\pi \alpha i + \phi) c_i^\dagger c_i,$$

where $c_i^\dagger (c_i)$ denotes the creation (annihilation) operator on a lattice site $i$, $\alpha$ is an irrational number, $J_{\text{AA}}$ is the site-independent tunneling, $\Delta_{\text{AA}}$ describes the strength of the onsite energies, and $\phi$ is an arbitrary phase. Here, we
FIG. 1. Precise quantum simulation of AA model. (a), The optical potential \( V_{D,\text{precise}} \) (red solid line) and \( V_{D,\text{err}} \) (blue dash-dotted line). The potential \( V_{D,\text{precise}} \) possesses a vanishing derivative at the individual sites (black dots), whereas \( V_{D,\text{err}} \) does not. (b), The onsite energies produced by \( V_{D,\text{precise}} \) (red circles) and \( V_{D,\text{err}} \) (blue crosses). The dashed line is the desired sinusoidal form of the site-dependent onsite energies in \( H_{\text{AA}}^* \). (c), The tunnelings produced by \( V_{D,\text{precise}} \) (red circles) and \( V_{D,\text{err}} \) (blue crosses). The dashed line marks the desired site-independent tunnelings in \( H_{\text{AA}}^* \). Here, we choose the high-band cutoff \( M_c = 2 \), the hyper-parameter \( \lambda_1 = 1 \), the system size \( L = 55 \), and periodic boundary condition.

choose \( \alpha \) as the golden ratio \((\sqrt{5} - 1)/2\), which is approximated by the Fibonacci sequence \((F_n)\) as \( F_n/F_{n+1} \) in a finite-size calculation. Because of its energy independent duality defined by a Fourier transform, the model exhibits a phase transition from all wave-function localized to all extended, which makes it natural place to examine one-dimensional localization criticality.

In the optical lattice experiment [16], the AA model Hamiltonian is achieved by using an incommensurate bichromatic potential, a primary lattice perturbed by a second weak incommensurate lattice with \( V_{D,\text{err}}(x) = V_1 \cos(2\alpha k x)/2 \) following our notation in Eq. 1. However, its corresponding tight-binding model is not a precise AA model—there are corrections making tunnelings inhomogeneous and generating higher-order harmonics, which generically breaks the central ingredient of duality of the AA model [49]. The effects of such corrections have been established both in theory [17] and experiment [18, 19]. This problem can be solved by using our precise quantum simulation method.

Through the optimization described above, we find that precise quantum simulation of AA model is achieved by choosing a potential

\[
V_{D,\text{precise}}(x) = \frac{V_1}{2} \cos \left( \frac{2}{F_n} F_{n+1} k x \right) + \frac{V_2}{2} \cos \left( \frac{2}{F_{n-1}} F_{n+1} k x \right),
\]

with appropriate coefficients \( V_{1,2} \). As an example, we consider a specific model \( H_{\text{AA}}^* \) with parameters \( J_{\text{AA}} = -0.0308 E_R \), \( \epsilon_{\text{AA}} = 0.0841 E_R \), \( \alpha = F_n/F_{n+1} (F_n = 34 \text{ and } F_{n+1} = 55) \), and \( \phi = -\pi \alpha \). This target model is reached by choosing \( V_p = 8 E_R \), \( V_1 = 0.1 E_R \), \( V_1 = 0.0341 E_R \), and \( V_2 = -0.0592 E_R \). In Fig. 1(a), we show the optical potentials corresponding to \( V_{D,\text{err}} \) and \( V_{D,\text{precise}} \) for comparison. We find that the resultant onsite energies are approximately the same (Fig. 1(b)), yet with the potential \( V_{D,\text{precise}} \) giving a more precise solution. More drastically, the tunnelings out of our potential with \( V_{D,\text{precise}}(x) \) are precisely homogeneous, with a relative inhomogeneity below \( 1E - 4 \) (Fig. 1(c)). This cannot be achieved with the potential of \( V_{D,\text{err}}(x) \).

We also emphasize here that our constructed potential \( V_{D,\text{precise}}(x) \) possesses a vanishing derivative at the individual sites, as exhibited in Fig. 1(a). This is crucial to experiments as a potential with finite derivative at the position of atoms would make the system more susceptible to shaking-induced heating processes [48].

Anderson localization with programmable disorder potential.— To further demonstrate the precise programmability enabled by our method, we also carry out an application to quantum simulation of Anderson localization models whose previous experimental realization by speckle pattern lacks programmability [22–33]. The Hamiltonians of 1D AL models are given as

\[
H_{\text{AL}} = \sum_i \hbar c_i^\dagger c_i + \sum_i \left( t_i c_{i+1}^\dagger c_i + h.c. \right).
\]

We consider three different cases: (a) random onsite model with \( h_i \in [-\bar{\epsilon}_{\text{AL}}/2, \bar{\epsilon}_{\text{AL}}/2] \) and \( t_i = J_{\text{AL}} \) being homogeneous, (b) random hopping model with \( h_i = \epsilon_{\text{AL}} \) homogeneous and \( t_i \in [J_{\text{AL}} - J_{\text{AL}}/2, J_{\text{AL}} + J_{\text{AL}}/2] \), and (c) both onsite energies and tunnelings being random with \( h_i \in [-\bar{\epsilon}_{\text{AL}}/2, \bar{\epsilon}_{\text{AL}}/2] \) and \( t_i \in [J_{\text{AL}} - J_{\text{AL}}/2, J_{\text{AL}} + J_{\text{AL}}/2] \). The random onsite energies and tunnelings are drawn according to a uniform distribution. In Fig. 2, we show all the three different cases of AL model can be precisely achieved with our optimization method. The absolute errors in the tight-binding model compared to the target one is made smaller than \( 1E - 5 \), which demonstrates the precise programmability of our scheme.

One immediate application of the programmable quantum simulation of Anderson localization is to study the anomalous localization in the random hopping model.
FIG. 2. Precise quantum simulation of three cases of AL models. (a), The random onsite model with $h_i \in [-0.05E_R, 0.05E_R]$ and $t_i = -0.0308E_R$ being homogeneous. (b), The random hopping model with $h_i = 0$ homogenous, $t_i \in [J_{AL} - |J_{AL}|/2, J_{AL} + |J_{AL}|/2]$, and $J_{AL} = -0.0308E_R$. (c), Both onsite energy and tunneling being random with $h_i \in [-0.05E_R, 0.05E_R]$, $t_i \in [J_{AL} - |J_{AL}|/2, J_{AL} + |J_{AL}|/2]$, and $J_{AL} = -0.0308E_R$. The first row shows the reverse-engineered optical potentials $V_D(x)$, the middle row and the last row shows the onsite energies and the tunnelings. Circles and crosses indicate the values in the tight-binding models extracted from the continuous Hamiltonian in Eq. (1) and the targeting tight binding model, respectively. Here, we choose the high-band cutoff $M_c = 2$, the hyper-parameter $\lambda_1 = 100$, the system size $L = 10$, and periodic boundary condition.

FIG. 3. Averaged IPR for the random hopping model (Eq. (7)) by sampling 2000 disorder configurations. Here we set $J_{AL} = -0.0308E_R$ and $J_{AL} = 2|J_{AL}|/3$, the system size $L = 100$. The blue solid, and red dash-dotted lines, correspond to the results obtained from diagonalizing the continuous Hamiltonian in Eq. (1) and the tight binding random-hopping model, respectively. Here, we choose the high-band cutoff $M_c = 2$, the hyperparameter $\lambda_1 = 100$, the system size $L = 100$, and periodic boundary condition. The whole system is split into a number of pieces with $L_p = 10$, and the adjacent pieces overlap with each other over 4 sites. We choose the hyper-parameter $\lambda_2 = 0.05$.

Unlike the random onsite model where all states are localized in one dimension, the random hopping model has delocalized states at band center [50, 51]. But it is extremely difficult to perform quantum simulation of this pure random hopping model with the speckle-pattern approach lacking programmability, since the unavoidable inhomogeneity in the onsite energy will make all states localized. We randomly generate 2000 disorder samples for the hopping, and compute the corresponding potential $V_D(x)$ using our optimization method. The averaged inverse participation ratio (IPR) which diagnoses localization to delocalization transition [52] is calculated, with the results shown in Fig. 3. We find quantitative agreement of results obtained for the continuous potential with the targeting tight-binding model. The discrepancy can be further improved by increasing the lattice depth or allocating more numerical resources.

We emphasize that the precise programmable quantum simulation enabled by our scheme make the optical lattice rather flexible. For disorder physics, having programmable disorder allows for more systematic study of the localization transition, especially for cases where the rare disorder Griffith effects are important for example in understanding disordered Weyl semimetals [53] and many-body localization mobility edge [54, 55]. Our
proposing setup also paves a way to building a programmable quantum annealer with optical lattices. Considering spinor atoms in a deep lattice with strong interaction, programmable tunnelings imply programmable spin-exchange. How to make the spin-exchange precisely programmable would require a Wegner flow of an interacting Hamiltonian, which is left for a future study.

Final remark.— We have proposed a scheme for precisely simulating lattice models with optical lattices, whose potentials can be manipulated through the high-resolution DMD techniques. We have developed a Wegner-flow method to extract the precise tight-binding model of a continuous potential, and a scalable optimization method for the reverse engineering of the optical potential whose tight binding model precisely matches a targeting model. The performance is demonstrated with concrete examples of AA and Anderson models. Our approach implies optical lattices can be upgraded towards high-precision programmable quantum simulations by integrating with DMD techniques.

Acknowledgement.— We acknowledge helpful discussions with Peter Zoller, Immanuel Bloch, and Yu-Ao Chen. This work is supported by National Natural Science Foundation of China under Grants No. 11934002, and National Program on Key Basic Research Projects of China under Grant No. 2017YFA0304204. Xingze Qiu acknowledges support from National Postdoctoral Program for Innovative Talents of China under Grant No. BX20190083.

* xiaopeng_li@fudan.edu.cn

[1] Altman, E. et al. Quantum simulators: Architectures and opportunities (2019). 1912.06938.
[2] Bloch, I., Dalibard, J. & Nascimbene, S. Quantum simulations with ultracold quantum gases. Nature Physics 8, 267–276 (2012).
[3] Georgescu, I. M., Ashhab, S. & Nori, F. Quantum simulation. Reviews of Modern Physics 86, 153 (2014).
[4] Gross, C. & Bloch, I. Quantum simulations with ultracold atoms in optical lattices. Science 357, 995–1001 (2017).
[5] Bloch, I. Quantum simulations come of age. Nature Physics 14, 1159–1161 (2018).
[6] Dalibard, J., Gerbier, F., Juzeliūnas, G. & Öhberg, P. Colloquium: Artificial gauge potentials for neutral atoms. Reviews of Modern Physics 83, 1523 (2011).
[7] Zhai, H. Degenerate quantum gases with spin–orbit coupling: a review. Reports on Progress in Physics 78, 026001 (2015).
[8] Zhang, L. & Liu, X.-J. Spin-orbit coupling and topological phases for ultracold atoms. Synthetic Spin-Orbit Coupling in Cold Atoms 187 (2018).
[9] Cooper, N., Dalibard, J. & Spielman, I. Topological bands for ultracold atoms. Reviews of Modern Physics 91, 015005 (2019).
[10] Regal, C., Greiner, M. & Jin, D. S. Observation of resonance condensation of fermionic atom pairs. Phys. Rev. Lett. 92, 040403 (2004).
[11] Greif, D., Uehlinger, T., Jotzu, G., Tarruell, L. & Esslinger, T. Short-range quantum magnetism of ultracold fermions in an optical lattice. Science 340, 1307–1310 (2013).
[12] Mazurenko, A. et al. A cold-atom fermi–hubbard antiferromagnet. Nature 545, 462–466 (2017).
[13] Hart, R. A. et al. Observation of antiferromagnetic correlations in the hubbard model with ultracold atoms. Nature 519, 211–214 (2015).
[14] Brown, P. T. et al. Bad metallic transport in a cold atom fermi-hubbard system. Science 363, 379–382 (2019).
[15] Trotzky, S. et al. Probing the relaxation towards equilibrium in an isolated strongly correlated one-dimensional bose gas. Nature Physics 8, 325–330 (2012).
[16] Schreiber, M. et al. Observation of many-body localization of interacting fermions in a quasirandom optical lattice. Science 349, 842–845 (2015).
[17] Li, X., Li, X. & Sarma, S. D. Mobility edges in one-dimensional bichromatic incommensurate potentials. Phys. Rev. B 96, 085119 (2017).
[18] Lüschen, H. P. et al. Single-particle mobility edge in a one-dimensional quasiperiodic optical lattice. Phys. Rev. Lett. 120, 160404 (2018).
[19] Kohlert, T. et al. Observation of many-body localization in a one-dimensional system with a single-particle mobility edge. Phys. Rev. Lett. 122, 170403 (2019).
[20] Harper, P. G. Single band motion of conduction electrons in a uniform magnetic field. Proceedings of the Physical Society. Section A 68, 874 (1955).
[21] Aubry, S. & André, G. Analyticity breaking and anderson localization in incommensurate lattices. Ann. Israel Phys. Soc 3, 18 (1980).
[22] Damski, B., Zakrzewski, J., Santos, L., Zoller, P. & Lewenstein, M. Atomic bose and anderson glasses in optical lattices. Phys. Rev. Lett. 91, 080403 (2003).
[23] Gavish, U. & Castin, Y. Matter-wave localization in disordered cold atom lattices. Phys. Rev. Lett. 95, 020401 (2005).
[24] Schulte, T. et al. Routes towards anderson-like localization of bose-einstein condensates in disordered optical lattices. Phys. Rev. Lett. 95, 170411 (2005).
[25] Billy, J. et al. Direct observation of anderson localization of matter waves in a controlled disorder. Nature 453, 891–894 (2008).
[26] White, M. et al. Strongly interacting bosons in a disordered optical lattice. Phys. Rev. Lett. 102, 055301 (2009).
[27] Sanchez-Palencia, L. & Lewenstein, M. Disordered quantum gases under control. Nature Physics 6, 87–95 (2010).
[28] Pasienski, M., McKay, D., White, M. & DeMarco, B. A disordered insulator in an optical lattice. Nature Physics 6, 677–680 (2010).
[29] Kondov, S., McGeehe, W., Zirbel, J. & DeMarco, B. Three-dimensional anderson localization of ultracold matter. Science 334, 66–68 (2011).
