Skin Superfluid, Topological Mott Insulators, and Asymmetric Dynamics in Interacting Non-Hermitian Aubry-André-Harper Models

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(Dated: January 22, 2020)

Non-Hermitian quantum many-body systems are a fascinating subject to be explored. Using the generalized density matrix renormalisation group method and complementary exact diagonalization, we elucidate the many-body ground states and dynamics of a 1D interacting non-Hermitian Aubry-André-Harper model for bosons. We find stable ground states in the superfluid and Mott insulating regimes under wide range of conditions in this model. We reveal a skin superfluid state induced by the non-Hermiticity from the nonreciprocal hopping. We investigate the topology of the Mott insulating phase and find its independence of the non-Hermiticity. The topological Mott insulators in this non-Hermitian system are characterized by four equal Chern numbers and a quantized shift of biorthogonal many-body polarizations. Furthermore, we show generic asymmetric expansion and correlation dynamics in the system.

Introduction.—Non-Hermitian systems have intriguing physics and applications beyond Hermitian systems [1–4]. Topological phases in noninteracting non-Hermitian systems have been widely studied [3,45]. Non-Hermitian many-body physics is expected to be a fascinating but much less explored area [47–63]. Notably, the interplay between non-Hermiticity and interactions can bring exotic quantum many-body effects, such as non-Hermitian extensions of Kondo effect [52,53], many-body localization [54], and fermionic superfluidity [55,56]. Topological states in one-dimensional (1D) interacting non-Hermitian Su-Schrieffer-Heeger model [54] and fractional quantum Hall system with non-Hermitian interactions are revealed [57,59]. However, these work mainly focus on static properties in the mean-field regime or small systems with few particles [47–63]. Interacting non-Hermitian systems of large sizes and their dynamics remain largely unexplored, which is partially due to the lack of efficient numerical tools for non-Hermitian quantum many-body systems. For instance, the density matrix renormalisation group (DMRG) [65–67] is one of the most powerful numerical methods for 1D strongly correlated Hermitian systems, but the convergence of the calculation is not guaranteed for a non-Hermitian Hamiltonian.

In this Letter, based on our generalized DMRG method and complementary exact diagonalization (ED), we elucidate the many-body ground states and quantum dynamics of a 1D interacting non-Hermitian Aubry-André-Harper (AAH) model [65,69] for bosons. This model has not been studied in previous work [47,63], probably because the usually used DMRG fails to study this model in the non-Hermitian case. We here first improve the DMRG approach and then investigate the many-body non-Hermitian AAH model and our main results for this model are as follows: (i) We uncover well-defined and stable ground states in the superfluid and Mott insulating phases in this non-Hermitian system under both open boundary conditions (OBCs) and periodic boundary conditions (PBCs). (ii) We reveal a skin superfluid state under OBCs induced by non-Hermiticity from the nonreciprocal hopping. (iii) We investigate the topological properties of the Mott insulating phase and find that the topological Mott insulators (TMIs) [70–74] independence of the non-Hermiticity. The TMIs in our non-Hermitian system are characterized by four equal Chern numbers defined under twisted PBCs and a quantized shift of biorthogonal many-body polarizations under OBCs. (iv) We show generic asymmetric expansion and correlation dynamics due to the nonreciprocal hopping in the system. The AAH model has been realized with (interacting) bosonic atoms in 1D optical superlattices [75–78] and the non-Hermiticity for cold atoms has been engineered [81]. Since combing these two ingredients is easily in current experiments, our results are observable. Moreover, our numerical methods can be used to explore non-Hermitian quantum many-body physics in both equilibrium and nonequilibrium cases.

Model and stable ground states.—We start by considering a 1D optical superlattice of interacting bosons [75,77] with nonreciprocal hoppings [82,83], which is described by the 1D interacting non-Hermitian AAH Hamiltonian

\[
H = -\sum_j (J_r \hat{a}_{j+1}^\dagger \hat{a}_j + J_l \hat{a}_j^\dagger \hat{a}_{j+1}) + V \sum_j \cos(2\pi \alpha_j + \delta) \hat{n}_j + \frac{U}{2} \sum_j (\hat{n}_j - 1),
\]

(1)

where \(\hat{a}_j^\dagger (\hat{a}_j)\) is the creation (annihilation) operator of bosons at site \(j\), \(\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j\) is the particle number operator, \(J_r\) and \(J_l\) are the nonreciprocal hopping strengths,
$V$, $\alpha$ and $\delta$ denote the modulation parameters of the superlattice, and $U$ is the on-site interaction strength. We focus on the periodic modulation with $\alpha$ being a rational number and the phase $\delta \in [0, 2\pi]$ acting as an effective quasimomentum in a synthetic dimension \([84–86]\). We set $J_{c} = J$ and $J_{f} = J(1 - \gamma)$, with the non-Hermiticity parameter $\gamma$ (let $\gamma \geq 0$) and $J = 1$ as the energy unit hereafter. When $\gamma = 0$, the Hamiltonian becomes Hermitian with topological insulating phases in the Mott regime \([71,72]\). When $U = 0$, the Hamiltonian reduces to the single-particle non-Hermitian AAH model with nontrivial topological properties \([43,44,87]\). The topological phases in this case can be characterized by nonzero Chern numbers (defined in the $k$-$\delta$ space with quasimomentum $k$ under PBCs) \([42,43]\). We find a quantized shift of biorthogonal polarizations with respect to $\delta$ under OBCs as another topological invariant \([67]\), which is naturally generalized to the interacting cases, as given in Eq. \((\ref{eq:gamma})\).

The complex energy spectrum $E_{n}$ and wave functions of the right (left) states $|\Psi_{n}^{R}\rangle$ ($|\Psi_{n}^{L}\rangle$) with $n = 0, 1, 2, \ldots$ can be obtained by solving the eigenfunction $\hat{H}|\Psi_{n}^{R}\rangle = E_{n}|\Psi_{n}^{R}\rangle$ ($\hat{H}^{\dagger}|\Psi_{n}^{L}\rangle = E_{n}^{*}|\Psi_{n}^{L}\rangle$), which are ordered by the real-part energies $\text{Re}(E_{n})$. The ground states have the minimum value of $\text{Re}(E_{n})$ and then the excitation gap can be defined as $\Delta_{\text{ex}} = \text{Re}(E_{1}) - \text{Re}(E_{0})$ for the non-degenerate ground state $|\Psi_{0}^{0}\rangle$ ($|\Psi_{0}^{L}\rangle$), as a natural extension of Hermitian systems. We numerically obtain $E_{n}$ for a lattice $L = 18$ (ED) with $\alpha = 1/3$ and the filling $f = N/L = 1/3$ with the particle number $N = 6$, with an example shown in Fig. \(\text{I(a)}\). Under OBCs, we find that all $E_{n}$ are purely real for any $U$ when $\gamma < 1$, which generally become complex when $\gamma > 1$. Thus, $\gamma = 1$ is the exceptional point with the parity-time symmetry breaking for the many-body ground state under OBCs, as shown in Fig. \(\text{I(b)}\). The result can be understood that there is a similarity transformation $S$ mapping the non-Hermitian Hamiltonian to a Hermitian counterpart $\hat{H}' = S\hat{H}S^{-1}$ under OBCs when $\gamma < 1$, where $S$ is a diagonal matrix in the Fock space and $\hat{H}'(J', V', U')$ denotes the corresponding Hermitian interacting AAH Hamiltonian with parameters $J' = J\sqrt{1 - \gamma}$, $V' = V$, and $U' = U$.

The same energy spectra of $\hat{H}$ and $\hat{H}'$ are confirmed in our numerical simulations. More interestingly, we find the eigenenergies of $\hat{H}$ under PBCs are complex conjugate pairs or real for any values of $\gamma$ and $U$ and in particular, $E_{0}$ is real in this case. This is guaranteed by the pseudo-Hermiticity of $\hat{H}$ under PBCs as it satisfies $I\hat{H}^{-1} = \hat{H}^{\dagger}$ \([88,89]\), where $I : \sigma_{3} \rightarrow \sigma_{L+1}$ is the inversion symmetry in this system. The non-degeneracy of $|\Psi_{0}^{R}\rangle$ ($|\Psi_{0}^{L}\rangle$) guarantees $E_{0}$ to be real. Thus, this interacting non-Hermitian system always has well-defined and stable many-body ground states with the real and smallest energy under OBCs with $\gamma < 1$ or under PBCs.

**Non-Hermitian DMRG.**— The DMRG method is powerful in the numerical calculation of the ground state of a 1D strongly correlated system \([65,66]\). For Hermitian systems, the convergence of the ground state calculation is mainly determined by the DMRG sweeps instead of the eigensolver in each variational update. However, due to the non-orthogonality of eigenstates in non-Hermitian matrices, the convergence usually fails by merely increasing the DMRG sweeps. We solve this convergence problem by using a more accurate eigensolver, the implicitly restarted Arnoldi method \([90]\), to target the ground state defined by the lowest real-part energy. We find that this non-Hermitian DMRG method can accurately obtain the energies and wave functions of many-body ground states. Furthermore, by generalizing the Krylov-subspace approach in Arnoldi formalism \([91]\) and the time-dependent variational principle (TDVP) method \([92,93]\), we can simulate the non-unitary time evolution (dynamics) in this model. The ingredients and benchmarks of these non-Hermitian algorithms are presented in the Supplemental Material \([67]\).

**Skin superfluid under OBCs.**— The many-body ground state of the interacting bosons is in the superfluid or Mott insulating phase with a critical interacting strength $U_{c}$. We now consider the superfluid state, which can be characterized by the one-particle density matrix. In the biorthogonal basis for this non-Hermitian system under PBCs, there are four components of the one-particle density matrix defined as $\rho_{ab} = \langle |\Psi_{0}^{R}\rangle|\tilde{a}_{L/2+1}^{\dagger}|\Psi_{0}^{L}\rangle$ for right and left ground states, with $a, b = \uparrow, \downarrow$. Here $\rho_{ab}$ captures the momentum distribution of the interacting bosons and is associated with an off-diagonal quasi-long-range order if $\rho_{ab}$ remains finite at large $L$. The typical results of $\rho_{ab}$ from the ED ($L = 18$) and the DMRG ($L = 90$) as a function of $U$ are shown in Fig. \(\text{II(a)}\). The four components $\rho_{ab}$ are real (here the slight differences among $\rho_{ab}$ are due to the modulation potential $V$) and indicate the superfluid (Mott insulating) phase for small (large) $U/J$, similar as those in Hermitian Bose-Hubbard models \([14]\).

The excitation gap can be used to determine the critical point $U_{c}/J$ (at zero temperature and in the thermodynamic limit) between the gapless superfluid phase and the gapped Mott insulating phase. For realistic systems under OBCs, the excitation gap $\Delta_{\text{ex}}$ for the non-Hermitian...
Hamiltonian $\hat{H}(J, U, V)$ can be obtained from that for the Hermitian counterpart $\hat{H}'(J', U, V)$ after the similarity transformation when $\gamma < 1$. Figure 2(b) shows the finite-size scaling of $\Delta_{ex}$ for various $U$ and $\gamma = 0.8$, which gives $U_c/J \sim 0.5$ through extrapolation to the $L \to \infty$ limit. Using this procedure, we numerically obtain $U_c/J$ as a function of the non-Hermiticity $\gamma$ for fixed $V/J = 1$ or $V/J' = 1$, as shown in Fig. 2(c). One can find that $U_c/J$ is decreased when increasing $\gamma$ and $U_c/J \propto \sqrt{1 - \gamma}$ for the case with fixed $V/J'$, which can be understood from the reduced effective reciprocal hopping $J' = J\sqrt{1 - \gamma}$ under OBCs.

In Fig. 2(d), we show the superfluid density distribution $n_j = \langle \Psi^\dagger_j \hat{n}_j \Psi_0 \rangle$ defined for the right ground state for different conditions. Under PBCs, we find that the superfluid density distribution is periodically modulated by the superlattice potential $V$, which is independent on $\gamma$ and will become nearly uniform when $V/J \ll 1$. Under OBCs, in contrast, the superfluid tends to localized at the right side of the lattice by increasing $\gamma$ ($0 \lesssim \gamma < 1$) due to the asymmetric hopping $J_J > J_l$. This can be understood as a many-body generalization of the non-Hermitian skin effect [10], and thus such a superfluid state under OBC is dubbed skin superfluid. Notably, the skin superfluid under OBCs is more significant for larger $\gamma$ and smaller $U/J$, and the potential $V$ just adds the overall modulation in the density distribution.

Non-Hermitian TMI: We proceed to investigate the topological properties of the Mott insulating phase. Figure 3(a) depicts that the excitation gap $\Delta_{ex}$ increases as a function of $U$ and saturates at a finite value for large $U$. Note that the nonzero value of $\Delta_{ex}$ for the superfluid phase in the small $U$ limit is actually the finite-size gap in the ED simulation. In the presence of a finite gap, we can use the Chern number to characterize the topology of the Mott insulators. For our non-Hermitian system, under the twisted PBCs with a twisted phase $\theta$ [95], we can define four Chern numbers in the $\theta$-$\delta$ space as

$$C_{ab} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \int_0^{2\pi} d\delta F_{ab}(\theta, \delta),$$

where $F_{ab}(\theta, \delta) = i\langle \hat{\partial}_\theta \Psi_0^b | \hat{\partial}_\delta \Psi_0^a \rangle$ is the four Berry curvatures related to the left and right many-body ground states. We calculate $C_{ab}$ by evaluating $F_{ab}$ using a discrete manifold method [71, 96, 97], and find that four Chern numbers are equal $C_{rr} = C_{ll} = C_{rt} = C_{lt} = C$ as a function of $U$ as shown in Fig. 3(a). This implies that the Chern number $C$ is invariant to different choices of right and left many-body ground states [21]. In the deep Mott insulator regime, such as $U = 10$, one has $C = 1$ indicating a TMI. Note that the Chern number is actually not well-defined for small $U$ although $C$ remains quantized in Fig. 3(a) due to the finite-size effect.

We find another topological invariant to characterize the TMI under OBCs, which is related to the biorthog-
FIG. 4: (Color online) Dynamics of one-particle density $G_1$ and two-particle correlation $G_2$ for the initial state with $N = 5$ bosons localized one per site in the center of a $L = 31$ lattice. (a-d) $G_1$ with zero and non-zero asymmetric hopping $\gamma$, and moderate and strong interaction strength $U$. (e-h) $G_2$ for the same parameters with respect to the upper panel (a-d).

for  the many-body ground state under OBCs, the expression of $\hat{P}$ for $L$ lattice sites and $N$ bosons is given by

$$\hat{P}(\delta) = \frac{1}{N} \sum_{j=1}^{L} j\langle \Psi^\dagger_0(\delta)|\hat{n}_j|\Psi_0(\delta)\rangle,$$

which is a function of the periodical modulation phase $\delta$. Figure 3(b) depicts the DMRG results of $\hat{P}(\delta)$ for $L = 3N = 90$, $\gamma = 0.2$ and $U = 10$. Here $\hat{P}$ exhibits a jump of nearly one unit cell (three sites) by varying $\delta$ from 0 to $2\pi$, corresponding to $C = 1$. So a quantized shift (when $L \rightarrow \infty$) of the biorthogonal many-body polarization under OBCs is also a topological invariant for our interacting non-Hermitian model.

The quasiparticle energy spectrum under OBCs can be obtained from the DMRG, which is real and given by $\delta E_N = E_{0,N+1} - E_{0,N}$. Here $E_{0,N}$ is the energy of the ground state with $N$ bosons denoted by $|\Psi_{0,N}^r\rangle$ and is real under OBCs ($\gamma < 1$). Figure 3(c) shows $\delta E_N$ as a function of $\delta$ near the filling $f = 1/3$ for $L = 90$. There are two branches of in-gap edge modes that are degenerate at $\delta = 2\pi/3$ and connect the lower and the upper bulk spectra when $\delta$ varies from 0 to $2\pi$, corresponding to the TMI with $C = 1$. The right-state and biorthogonal density distributions of quasiparticles are respectively given by $\delta\eta_j = \langle \Psi^\dagger_{0,N+1}|\hat{n}_j|\Psi_{0,N+1}\rangle - \langle \Psi^\dagger_{0,N}|\hat{n}_j|\Psi_{0,N}\rangle$ and $\delta\tilde{n}_j = \langle \Psi^\dagger_{0,N+1}|\hat{n}_j|\Psi_{0,N+1}\rangle - \langle \Psi^\dagger_{0,N}|\hat{n}_j|\Psi_{0,N}\rangle$. The results of $\delta\eta_j$ and $\delta\tilde{n}_j$ for the two degenerate edge modes at $\delta = 2\pi/3$ are shown in Fig. 3(d). Due to the asymmetric hopping for the right eigenstates, $\delta\eta_j$ for the two edge modes exhibit asymmetric distributions. The asymmetric hopping is cancelled under the biorthogonal eigenstates and then $\delta\tilde{n}_j$ for the two edge modes remain symmetric distributions.

We further study the non-Hermitian effect on the TMI. Figure 3(c) shows that the obtained Chern number is independent on the non-Hermiticity $\gamma$. Remarkably, it preserves even when $\gamma > 1$ as the ground state still has a finite gap in the complex energy plane under PBCs. Thus, although the many-body energy spectrum is generally complex, the non-Hermitian TMI in this system can still be topologically connected to the Hermitian TMI with $\gamma = 0$. This can be understood that 1D interacting non-Hermitian systems share the same topological classification as that of the Hermitian systems $[57]$. We further confirm that the Chern number and the stable ground states with real energies preserve in the large $L$ limit from the DMRG, as shown in Fig. 3(f).

Asymmetric dynamics.—Based on the TDVP method, we can study the dynamics in 1D non-Hermitian many-body systems $[67]$. We find that the nonreciprocal hopping can induce asymmetric expansion and correlation dynamics in this system. We consider the time-evolution of the one-particle density $G_1(j,t) = \langle \Psi^r(t)|\hat{a}_j^\dagger \hat{a}_j|\Psi^r(t)\rangle$ and the two-particle correlation function $G_2(q,p,t) = \langle \Psi^r(t)|\hat{a}_q^\dagger \hat{a}_p\hat{a}_p^{\dagger}\hat{a}_q|\Psi^r(t)\rangle$ $[68]$ to show the generic asymmetric dynamics, which are defined for the right states $|\Psi^r(t)\rangle$. Note that $G_1$ and $G_2$ (related to the density-density correlation) are both measurable for ultracold bosons in optical lattices. Typically, we consider the initial state $|\Psi^r(0)\rangle$ as a product state in the Fock space with $N = 5$ bosons localized at the center five sites of a lattice with $L = 31$. The system is then driven by the non-Hermitian Hamiltonian $H$ in Eq. 1.

The time-evolved state $|\Psi^r(t)\rangle = e^{-iHt}|\Psi^r(0)\rangle$ is calculated with the TDVP method with $J = 1$ and $V = 0$. We fix the lattice site $p = 16$ at the center of the lattice and then rewritten the two-particle correlation $G_2(d,t) = \langle \Psi^r(t)|\hat{a}_p^{\dagger}\hat{a}_p\hat{a}_p^{\dagger}\hat{a}_p\hat{a}_p^{\dagger}|\Psi^r(t)\rangle$ by introducing the distance $d = q - p$. The expansion dynamics of $G_1$ and the correlation dynamics of $G_2$ for zero and non-zero asymmetric hopping $\gamma$ and two interaction strengths $U$ are shown in upper and lower panels of Fig. 4, respectively. In the absence of asymmetric hopping $\gamma$ [Figs. 4(a,c,e,g)], the dynamics of both $G_1$ and $G_2$ are symmetric with respect to the center of the lattice. For the non-Hermitian cases, the one-particle density $G_1$ prefers to
propagate to the right-hand side of the lattice [Figs. 4 (b,d)] as the hopping $J_r > J_l$. This preference can be observed in the superfluid and Mott insulating phases for the two calculated interacting strengths. Similar asymmetric dynamics occur in the two-particle correlation $G_2$ [Figs. 4 (f,h)]. At the same time $t$, $G_2$ for $d > 0$ enjoys larger value than that for $d < 0$. It means that it is more likely to detect particles simultaneously at the center and right-hand side of the lattice than that at the left-hand side. Notably, the asymmetric expansion and correlation dynamics are absent under the biorthogonal eigenstates since the asymmetric hopping is cancelled in this basis.

**Conclusion.**—In summary, we have explored the stable many-body ground states and dynamics in the interacting non-Hermitian AAH model. We have revealed the nonreciprocal-hopping-induced skin superfluid under OBCs and the TMIs independence of non-Hermiticity. The TMIs are characterized by four equal Chern numbers and a quantized shift of biorthogonal many-body polarizations. We have shown generic asymmetric expansion and correlation dynamics due to the nonreciprocal hopping in this system. The AAH model can be realized with interacting ultracold bosons in 1D optical superlattices and the effective nonreciprocal hopping can be engineered by an atomic one-body loss. Thus, our predicted results could be observed in cold atom experiments. Furthermore, our numerical methods are applicable to explore non-Hermitian quantum many-body physics in both equilibrium and nonequilibrium cases.

This work was supported by the NSFC (Grants No. 11704367, No. 11904109, No. 91636218, No. U1830111, and No. U1801661), the NKRDP of China (Grant No. 2016YFA0301800), the Key-Area Research and Development Program of GuangDong Province (Grant No. 2019B030330001), and the Key Program of Science and Technology of Guangzhou (Grant No. 201804020055).

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Supplemental Materials

A. Single particle analysis

In the non-interacting limit, our Hamiltonian (Eq. (1) of the main text) becomes

\[ \hat{H}_0 = -\sum_j (J_j \hat{a}_j^\dagger \hat{a}_{j+1} + J_{j+1} \hat{a}_{j+1}^\dagger \hat{a}_j) + V \sum_j \cos(2\pi\alpha j + \delta) \hat{n}_j, \]

which is actually a single-particle non-Hermitian AAH model. The \( n \)-th eigenstate of the model is given by \( |\Psi_n^r\rangle = \sum_j u_{j,n} \hat{c}_j^\dagger |0\rangle \). We substitute it into the eigenvalue equation \( \hat{H}_0 |\Psi_n^r\rangle = E_n |\Psi_n^r\rangle \), then we obtain the following Harper equation

\[ -(J_j u_{j+1,n} + J_{j+1} u_{j-1,n}) + V_j u_{j,n} = E_n u_{j,n}, \]

where \( u_{j,n} \) is the wave function at the \( j \)-th site with the \( n \)-th eigenenergy \( E_n \). We consider the commensurate case where the parameter \( \alpha \) is rational. In this case, the superlattice potential \( V_j \) is periodic with a period \( q \) and the wave function satisfies \( u_{j,q} = e^{ikq} u_j \). Suppose \( \psi_j(k) (j = 1, \ldots, q) \) is the wave function in the momentum space and we take \( u_j = e^{ikj} \psi_j(k) \) for \( k \in [-\pi/q, \pi/q] \), then the Harper equation Eq. (5) becomes

\[ -(J_j e^{ik} \psi_{j+1} + J_{j+1} e^{-ik} \psi_{j-1}) + V_j \psi_j = E(k) \psi_j. \]

Under PBCs, we can get the eigenenergies and eigenstates by diagonalize the following matrix

\[
\begin{bmatrix}
V_1 & J_1 e^{-ik} & 0 & \cdots & J_{J_1} e^{ik} \\
J_1 e^{ik} & V_2 & J_2 e^{-ik} & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & J_{J_e} e^{-ik} & V_{J_e-1} & J_{J_e} e^{ik} \\
J_{J_e} e^{ik} & \cdots & 0 & J_{J_e} e^{ik} & V_{J_e}
\end{bmatrix}
\]

In Fig. 5, we plot the energy spectra in the complex plane for all \( \delta \) from 0 to \( 2\pi \) with \( \alpha = 1/3 \) under PBCs. We show the real part of the energy spectrum which consists of three bands in Fig. 5(a). In addition, there are non-zero imaginary part of the energy of the non-Hermitian AAH model, as shown in Fig. 5(b). Since the energy spectrum is separated in the complex plane, Chern number is still well-defined for this non-Hermitian system. Notably, we find that the Chern number is quantized to be exactly 1 for the occupied band. For OBCs, we calculate the eigenenergy and the biorthogonal polarization of the system. The biorthogonal polarization is given by the center of mass of the states at site \( j \) is calculated in the biorthogonal basis. As shown in Figs. 5(d) and 5(e), the non-Hermitian system has real energy spectrum under OBCs and the edge modes appear in the gapped regime. We also see the biorthogonal polarization \( P \) exhibits a change of nearly one unit cell when \( \delta \) varies from 0 to \( 2\pi \) in Fig. 5(f). Indeed, the change of the biorthogonal polarization is proportional to the Chern number.

B. Numerical methods and benchmarks

The DMRG is one of the most powerful numerical methods for 1D strongly correlated systems \cite{White1989,White1993}. In the following of this section, we discuss the technical ingredients of the non-Hermitian DMRG and TDVP methods and benchmark the flexibility of these numerical methods for the system we investigated, which has real or complex ground state energy at different parameters. Let us begin with the matrix product state (MPS) representation of a general 1D quantum state \( |\Psi\rangle \):

\[ |\Psi\rangle = \sum_{j_1, \ldots, j_L} \sum_{a_0, a_1, \ldots, a_L} \text{Tr}(M_{a_0, a_1}^{j_1} M_{a_1, a_2}^{j_2} \cdots M_{a_{L-2}, a_{L-1}}^{j_{L-1}} M_{a_{L-1}, a_L}^{j_L}) |j_1, j_2, \ldots, j_{L-1}, j_L\rangle. \]

Each \( M_{a_{n-1}, a_n}^{j_n} \) is a rank three tensor with \( j_n \) standing for the index of a local state, and \( a_n \) is a virtual index which connects adjacent sites (we will omit virtual indices for the sake of simplicity). For the open boundary condition, \( a_0 \)
and \( a_L \) are dummy indices and the trace operation is not needed. There exists a gauge freedom and one can bring MPS into canonical form:

\[
|\Psi\rangle = \sum_{\alpha=1}^{\chi_n} \Lambda^{[n]}_{\alpha} |l^{[n]}_\alpha\rangle |r^{[n]}_\alpha\rangle ,
\]

where \( n \) is the canonical center, \( \Lambda^{[n]} \) is a diagonal matrix containing the Schmidt values of the bipartition \( \{ l, r \} \), \( \chi_n \) is the total number of Schmidt values kept, \( |l^{[n]}_\alpha\rangle = \sum_j (A^{j_1} \cdots A^{j_n})_\alpha |j_1, \cdots, j_n\rangle \) and \( |r^{[n]}_\alpha\rangle = \sum_j (B^{j_{n+1}} \cdots B^{j_L})_\beta |j_{n+1}, \cdots, j_L\rangle \) are the orthonormal Schmidt states of the left and right parts respectively, and \( A^{j_i} (B^{j_L}) \) is the left (right) canonical form of the \( M^{j_i} \) tensor at site \( i \). The two-site DMRG method converges to the ground state \( |\Psi_0\rangle \) by variationally optimizing two neighboring MPS tensors \( M^{j_n,j_{n+1}} = A^{j_n} \Lambda^{[n]} B^{j_{n+1}} \) at once and minimize the energy \( \langle \Psi_0 | H | \Psi_0 \rangle \). The simply roadmap of the two-site algorithm is as follows [66]:

1. Prepare the MPS wavefunction \( |\Psi_0\rangle \) with canonical center at site \( n \):

\[
|\Psi_0\rangle = \sum_{\alpha,j_n,j_{n+1}: \beta} M^{j_n,j_{n+1}} |l^{[n-1]}_\alpha\rangle |j_n\rangle |j_{n+1}\rangle |r^{[n+1]}_\beta\rangle .
\]

In the variational update, tensors belong to \( |l^{[n-1]}\rangle \) and \( |r^{[n+1]}\rangle \) are fixed and \( M^{j_n,j_{n+1}} = A^{j_n} \Lambda^{[n]} B^{j_{n+1}} \) should be improved.

2. Generate the effective Hamiltonian \( \tilde{H}_{\text{eff}} \) under the projected basis \( |l^{[n-1]}_{\alpha,j_n,j_{n+1}} r^{[n+1]}_{\beta}\rangle \).

3. Numerically find the lowest lying eigenvector \( \tilde{M}^{j_n,j_{n+1}} \) of the effective Hamiltonian \( \tilde{H}_{\text{eff}} \).

4. (Sweep from left) Update tensor \( A^{j_n} = \tilde{A}^{j_n} \) on sites \( n \) from the singular value decomposition (SVD) of \( \tilde{M}^{j_n,j_{n+1}} = \tilde{A}^{j_n} \tilde{\Lambda}^{[n]} \tilde{B}^{j_{n+1}} \), prepare tensor \( M^{j_{n+1},j_{n+2}} = \tilde{\Lambda}^{[n]} \tilde{B}^{j_{n+1}} B^{j_{n+2}} \) for the next pair of sites.

(Sweep from right) Update tensor \( B^{j_{n+1}} = \tilde{B}^{j_{n+1}} \) on sites \( n+1 \) from the singular value decomposition of \( \tilde{M}^{j_n,j_{n+1}} = \tilde{A}^{j_n} \tilde{\Lambda}^{[n]} \tilde{B}^{j_{n+1}} \), prepare tensor \( M^{j_{n-1},j_n} = A^{j_{n-1}} \tilde{A}^{j_n} \tilde{\Lambda}^{[n]} \) for the next pair of sites.

5. Return to step 2 and sweep through the whole system till convergence.

FIG. 5: (Color online) (a)-(e) Energy spectra of the single-particle non-Hermitian AAH model with \( V = 1, \gamma = 0.2 \) and \( \alpha = 1/3 \). (a) The real and (b) imaginary part of the energy bands under PBCs. (c) The energy spectrum in the complex plane under PBCs. (d) The real and (e) imaginary part of the energy spectrum under OBCs as a function of \( \delta \) with \( L = 300 \). (f) The biorthogonal polarization \( P \) as a function of \( \delta \) under OBCs.
The non-orthogonality of a general matrix requires a more accurate eigensolver in step 3 of the non-Hermitian DMRG method and we implement a complex general version of the implicitly restarted Arnoldi (IRA) method similar to the widely used ARPACK package [99]. In practice, the IRA method only requires the action of\( \hat{H}_{\text{eff}} \) on a vector, and steps 2 and 3 are combined to avoid an explicit computation and storage of the effective Hamiltonian\( \hat{H}_{\text{eff}} \) which will significantly reduce the performance of the algorithm. The IRA method is set to target the eigenvalue with smallest real part in the spectrum, and typically \( 3 \sim 5 \) Arnoldi basis vectors and a strict energy toleration are used during numerical simulations.

In Figs. 6 (a) and (b), we plot the real and imaginary parts of the targeted ground state energy error \( \Delta E_0 \) for the 1D interacting non-Hermitian AAH Hamiltonian during the non-Hermitian DMRG sweeps, respectively. The energy error is defined as the difference between the previous energy \( E_0 \) and current energy \( E_0 \) reported by the DMRG algorithm: \( \Delta E_0 = E_0' - E_0 \). For strong interacting strength \( U = 10 \), the non-Hermitian DMRG method can quickly converge in a lattice of \( L = 90 \) lattice, and for moderate interacting strength \( U = 4 \), it also has good convergence in a lattice of \( L = 45 \). In this benchmark, a moderate \( L \) can converge even for a very large non-Hermitian parameter \( \gamma = 0.8 \). The reachable lattice size for small \( U \) is restricted because the energy gap between the ground state and excited state becomes difficult to distinguish in the variational optimization. In all cases benchmarked, asymmetric hopping strengths \( \gamma = 0.2, \gamma = 0.4, \text{and } \gamma = 0.8 \) show zero imaginary parts during the DMRG sweeps. We also benchmark systems with non-zero imaginary ground state energy and present results in Figs. 6 (d) and (e), where the nonreciprocal hopping strengths \( J_L = e^{i\gamma}J \) and \( J_L = e^{i\gamma}J \). Parameters are chosen the same as Figs. 6 (a,b) and both real and imaginary parts converge to \( \Delta E_0 = 10^{-12} \) for all cases.

The TDVP method is similar to the DMRG implementation except the third step [92], where eigensolver is replaced by the application of matrix exponential on the local wavefunction: \( M^{J_{n+1}J_{n+2}} = \exp(-i\hat{H}_{\text{eff}}\tau)M^{J_{n+1}J_{n+2}} \) with a small time step \( \tau \). There needs an addition operation in step 4 after the SVD, backward evolution of \( \tilde{\Lambda}^{[n]}B^{J_{n+1}} \) (when sweeping from left) or \( \tilde{\Lambda}^{[n]}A^{[n]} \) (when sweeping from right) before preparing the tensor \( M^{J_{n+1}J_{n+2}} \) or \( M^{J_{n-1}J_{n}} \) and this operation is actually similar to step 3 with time step \( -\tau \) and a different effective Hamiltonian [92]. By sweeping from \( n = 1 \) to \( n = L - 1 \), the initial wavefunction \( |\Psi(0)\rangle \) is involved to \( |\Psi(\tau)\rangle \), and long time involved wavefunction can be obtained by repeated sweeps along the lattice. In the non-Hermitian version, the wavefunction after each sweep needs normalization because the evolution operator \( \exp(-i\hat{H}_{\text{eff}}\tau) \) is not unitary. In practice, we employ the Krylov-subspace approach in Arnoldi formalism [101] and combine step 2 and 3 in a matrix free style to apply the non-Hermitian effective Hamiltonian matrix exponential on the local wavefunction. Figure. 6 (c) shows comparison
of numerical results of the expected occupation $n_c(t) = \langle \Psi^r(t)|\hat{n}_c|\Psi^r(t)\rangle$ obtained from the ED and TDVP methods with $c = 11$ as the central site of a $L = 21$ lattice. The initial state $|\Psi^r(0)\rangle$ is prepared in a product state where $N = 3$ bosons locate in the center of the lattice. The relaxation of $n_c$ obtained from the ED (asterisk points) and TDVP (solid curves) methods consistent with each other for all parameters simulated. The system for $J_r = J$ and $J_l = e^{i\gamma}J$ with complex energy spectrum is also simulated and displayed in Fig. 6 (f).

Our implementation of the non-Hermitian DMRG and TDVP algorithms is based on the ITensor library [100] and the demonstration codes can be found at https://github.com/PhyRespo/ITensor