Absence of topology in Gaussian mixed states of bosons

Christopher D. Mink, Michael Fleischhauer, and Razmik Unanyan
Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

(Received 20 February 2019; revised manuscript received 31 May 2019; published 25 July 2019)

In a recent paper [Bardyn *et al.*, Phys. Rev. X **8**, 011035 (2018)], it was shown that the generalization of many-body polarization to mixed states can be used to construct a topological invariant that is also applicable to finite-temperature and nonequilibrium Gaussian states of lattice fermions. The many-body polarization defines an ensemble geometric phase that is identical to the Zak phase of a fictitious Hamiltonian, whose symmetries determine the topological classification. Here we show that in the case of Gaussian states of *bosons*, the corresponding topological invariant is always trivial. This also applies to finite-temperature states of bosons in lattices with a topologically nontrivial band structure. As a consequence, there is no quantized topological charge pumping for translationally invariant bulk states of noninteracting bosons.

DOI: 10.1103/PhysRevB.100.014305

I. INTRODUCTION

Topological states of matter have fascinated physicists for many decades as they can give rise to interesting phenomena such as protected edge states and edge currents [1], quantized bulk transport in insulating states [2–7], and exotic elementary excitations [8–10]. Recently, several attempts were made to generalize the concept of topology to finite temperatures and to nonequilibrium steady states of noninteracting fermion systems [11–18]. This has been done for fundamental reasons and because of the intrinsic robustness of steady states of driven, dissipative systems. These systems are characterized by integer quantized topological invariants such as the winding of the Berry or Zak phase [19–22] or the Chern number leading to quantized observables in insulating states. Famous examples for this are the charge transport in a Thouless pump [4,6,23] or the Hall conductivity in Chern insulators [2,3,7,8]. For finite temperatures or under nonequilibrium conditions, these quantities are no longer quantized [24]. Furthermore, defining single-particle invariants becomes difficult as the system is in general in a mixed state. While for one-dimensional systems generalizations of geometric phases to density matrices based on the Uhlmann construction [25] can be used [13,15], their application to higher dimensions [14] is faced with difficulties [26].

In a recent paper [18], it was shown that the winding of the many-body polarization introduced by Resta [27] upon a closed path in parameter space is an alternative and useful many-body topological invariant for Gaussian states of fermions. The polarization of a nondegenerate ground state $|\psi\rangle$ corresponding to a filled band of a lattice Hamiltonian with periodic boundary conditions is the phase (in units of 2π) induced by a momentum shift $\hat{T}$,

$$P = \frac{1}{2\pi}\,\mathrm{Im}\ln\langle\psi|\hat{T}|\psi\rangle. \tag{1}$$

$\hat{T}$ shifts the lattice momentum $p_k = 2\pi k/L$ of all particles by one unit, $\hat{T}^{-1}\hat{c}_{\alpha,k}\hat{T} = \hat{c}_{\alpha,k+1}$, where L is the number of unit cells and α is a band index. As shown by King-Smith and Vanderbilt [28], expression (1) for a filled Bloch band is identical to the geometric Zak phase ϕ_{Zak} of this band. The amplitude of $z = \langle\psi|\hat{T}|\psi\rangle$, called the polarization amplitude, has been used as an indicator for particle localization [27,29,30]. For an insulating many-body state, $|z|$ remains finite in the thermodynamic limit of infinite particle number $N \to \infty$, while it vanishes in a gapless state [31,32].

P can straightforwardly be generalized to mixed states ρ and defines the ensemble geometric phase (EGP) ϕ_{EGP}:

$$\phi_{\mathrm{EGP}} = \mathrm{Im}\ln\mathrm{Tr}\{\rho\hat{T}\}. \tag{2}$$

Since mixed states are in general not gapped, $|\mathrm{Tr}\{\rho\hat{T}\}|$ is expected to vanish in the thermodynamic limit. However, ϕ_{EGP} remains well defined and meaningful for arbitrarily large but finite systems [18] as long as the so-called purity gap of ρ does not close. Furthermore, as shown in [18], the EGP of a Gaussian density matrix is reduced to the ground-state Zak phase of a *fictitious* Hamiltonian in the thermodynamic limit $L \to \infty$. The symmetries of this fictitious Hamiltonian determine the topological classification [12] following the scheme of Altland and Zirnbauer [33–35]. A phase transition between different topological phases occurs when the gap of the fictitious Hamiltonian closes for any finite system, i.e., when $|\mathrm{Tr}\{\rho\hat{T}\}| = 0$. The many-body polarization is a measurable physical quantity [18] and its quantized winding has direct physical consequences. For example, it can induce quantized transport in an auxiliary system weakly coupled to a finite-temperature or nonequilibrium system [36]. It should be noted, however, that due to the absence of a many-body gap, there is in general no adiabatic following in time, and the notion of adiabaticity has to be adapted [18].

Since the gapfulness of the many-body state is no longer given at finite temperatures, the question arises of whether the fermionic character of particles is of any relevance and if bosonic Gaussian systems can show nontrivial topological properties as well. In the present paper, we show rigorously that topological invariants based on many-body polarization are always trivial for Gaussian states of bosons. As a consequence, there is, e.g., no protected quantized charge pump

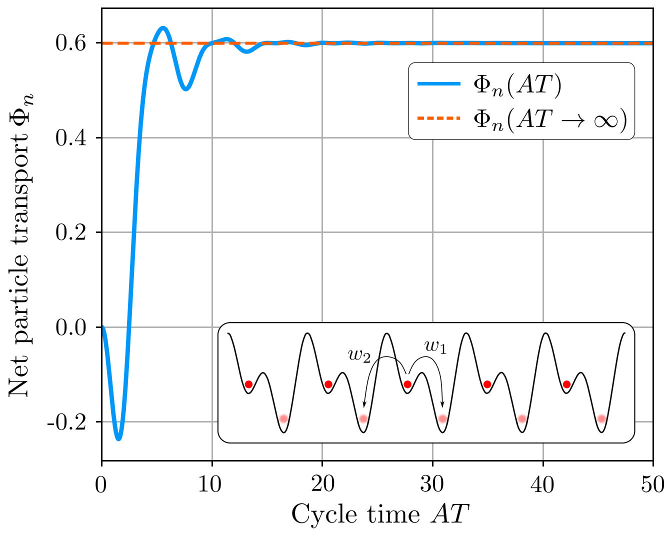

FIG. 1. Net particle transport as a function of the rescaled cycle time AT. Inset: Bosonic analog of the Rice-Mele model. Noninteracting bosons hop between neighboring lattice sites with alternating hopping rates w_1 and w_2. The on-site energies are shifted by $\pm\Delta$ in an alternating fashion.

for bosons under periodic, adiabatic variations of system parameters.

II. THE BOSONIC RICE-MELE MODEL

Bloch Hamiltonians with a topologically nontrivial band structure can lead to nontrivial many-body invariants of noninteracting fermions if all single-particle states of the corresponding band(s) are filled. In such states, the many-body polarization can show, e.g., a nontrivial winding under cyclic parameter variations. Surprisingly, the latter property survives at finite temperatures, i.e., even if the considered band is no longer fully occupied. Therefore, one may ask whether the many-body polarization can also show nontrivial behavior in the case of noninteracting *bosons*.

To illustrate what happens in such a case, let us consider one of the simplest 1D lattice models with single-particle topological properties, namely the Rice-Mele model (RMM) [23]. It has a unit cell consisting of two lattice sites with different on-site energies $\pm\Delta$, and it describes the hopping of particles with alternating hopping amplitudes $w_{1/2}$ (see the inset of Fig. 1). The Hamiltonian reads

$$\begin{aligned} H = -w_1 \sum_j \hat{a}_j^\dagger \hat{b}_j - w_2 \sum_j \hat{a}_{j+1}^\dagger \hat{b}_j + h.a. \\ + \Delta \sum_j (\hat{a}_j^\dagger \hat{a}_j - \hat{b}_j^\dagger \hat{b}_j), \end{aligned} \tag{3}$$

where $\hat{a}_j, \hat{b}_j$ are particle annihilation operators at the two sites of the jth unit cell, and we assume periodic boundary conditions. This model is well-known to have a nontrivial winding of the Zak phase [21],

$$\phi_{\text{Zak}} = \int_{\text{BZ}} dk \, \langle u_n(k)|\partial_k|u_n(k)\rangle, \tag{4}$$

of any one of the two subbands $n = 1, 2$ upon cyclic variations of the parameters $\Delta, w_1 - w_2$ encircling the origin $(\Delta = 0, w_1 = w_2)$ where the band gap closes. Here $|u_n(k)\rangle$ are the single-particle Bloch states of the nth band at lattice momentum $k2\pi/L$. Performing such a loop adiabatically, one can induce bulk transport if one subband is filled with fermions. At the same time, the many-body polarization also shows a nontrivial winding that, as shown by King-Smith and Vanderbilt, is strictly connected to the winding of ϕ_{Zak} [28].

Let us now consider the bosonic analog of the RMM. If initially only one unit cell is occupied, the center of mass of the wave packet moves by exactly one unit cell after a full cycle. This is because this particular initial state has equal amplitudes in all momentum eigenmodes of the band. The situation is very different, however, when we consider a translationally invariant, periodic system, where the many-body state returns to itself after a full cycle modulo a phase factor. Due to translational invariance, the Hamiltonian factorizes in momentum modes $\hat{a}_k, \hat{b}_k$,

$$H = \sum_k (\hat{a}_k^\dagger, \hat{b}_k^\dagger) \mathbf{h}_k(t) \begin{pmatrix} \hat{a}_k \\ \hat{b}_k \end{pmatrix}, \tag{5}$$

where $\mathbf{h}_k(t) = \boldsymbol{Q}_k(t) \cdot \boldsymbol{\sigma}$ is a 2×2 matrix describing a spin-$\frac{1}{2}$ particle in a magnetic field,

$$\boldsymbol{Q}_k(t) = \begin{pmatrix} w_1(t) + w_2(t) \cos\left(\frac{2\pi k}{L}\right) \\ w_2(t) \sin\left(\frac{2\pi k}{L}\right) \\ \Delta(t) \end{pmatrix}. \tag{6}$$

The spectrum of $\mathbf{h}_k(t)$ has two bands, $\epsilon_\pm(k, t) = \pm\epsilon_k(t)$, where $\epsilon_k(t) = [\Delta^2(t) + |w_1(t) + w_2(t) \exp(\frac{2i\pi k}{L})|^2]^{1/2}$. The system is assumed to start its evolution at $t = 0$, initially being in a (multimode) coherent state. Since the Hamiltonian is quadratic, the state remains a coherent state at all times. Specifically, we consider the initial state

$$|\Psi(0)\rangle = \underbrace{|\alpha\rangle|\beta\rangle}_{\text{Cell 1}} \otimes \cdots \otimes \underbrace{|\alpha\rangle|\beta\rangle}_{\text{Cell } L}, \tag{7}$$

with $|\alpha|^2 + |\beta|^2 = 1$, i.e., all cells are occupied equally with an average occupation of one per unit cell. We note that for coherent states, the particle number does not have a well-defined value. Furthermore, in contrast to the case of noninteracting fermions, this state corresponds to an initial occupation of only the $k = 0$ mode. Since the bosons are noninteracting, all initially empty modes ($k \neq 0$) remain empty during the time evolution. Thus, to describe the dynamics of the system, it is sufficient to consider only the $k = 0$ mode.

Let us now consider the number of particles transported after a full period T. The transport can be characterized in terms of the integrated particle flux, e.g., between the nth and $n + 1$st unit cell,

$$\Phi_n = i \int_0^T dt \, w_2(t) \langle\Psi(t)|(\hat{a}_{n+1}\hat{b}_n^\dagger - \hat{a}_{n+1}^\dagger \hat{b}_n)|\Psi(t)\rangle. \tag{8}$$

Due to the translational symmetry of the flux, Φ_n does not depend on n. Assuming that the initial amplitudes α and β coincide with an eigenstate of the Hamiltonian $\mathbf{h}_0$, and slowly varying the Hamiltonian parameters in time compared to the inverse energy gap $1/[2\varepsilon_{k=0}(t)]$, leads to an adiabatic following of the many-body state. Making use of the adiabatic approximation, after a straightforward calculation, we find for the integrated particle flux

$$\Phi_n = \frac{1}{2}\oint_{\mathcal{C}} \frac{w_1 + w_2}{\Delta^2\sqrt{\Delta^2 + (w_1 + w_2)^2}}(\Delta dw_2 - w_2 d\Delta), \tag{9}$$

where $\mathcal{C}$ is a closed path in the parameter space (w_1, w_2, Δ). One recognizes that the flux Φ_n can also be evaluated using Stokes' theorem by expressing it as an integral of a vector $\mathbf{B} = (w_1, w_2, \Delta)/[(w_1 + w_2)^2 + \Delta^2]^{3/2}$ through an area element $d\mathbf{S}$ in this parameter space $\Phi_n = \frac{1}{2}\int_{\mathcal{S}} \mathbf{B}\cdot d\mathbf{S}$, where $\mathcal{S}$ is a surface with boundary $\mathcal{C}$. Hence, after an integer number of cycles there is a net particle geometric transport, which is, however, not quantized (topological).

To be specific, we have shown in Fig. 1 the integrated particle current as a function of the rescaled cycle time AT with hopping rates $w_1(t) = A\cos^2(\frac{\pi t}{T})$, $w_2(t) = A\sin^2(\frac{\pi t}{T})$, and $\Delta(t) = A\sin(\frac{2\pi t}{T})$. The horizontal dashed line shows the adiabatic value

$$\Phi_n = \frac{1}{2}\int_0^{\pi} \frac{\cos^2(t)}{[\sin^2(t) + 1]^{3/2}} dt = \frac{\Gamma\left(\frac{3}{4}\right)}{\sqrt{2\pi}} \approx 0.6 \tag{10}$$

of the net particle transport.

While the particle transport is in general not quantized, the polarization (1) can only change by an integer-valued amount upon a full cycle of evolution, since it is the phase of a complex function (modulo 2π), provided there are no transitions to other states. The latter is guaranteed by the adiabatic evolution. In the above case, one finds that the polarization winding of the bosonic Rice-Mele model vanishes. In fact, one can easily calculate the polarization at any time t exactly. Fixing the gauge, i.e., fixing the origin of the spatial coordinate on the circle of length L, one obtains

$$P = \frac{1}{2\pi}\arg[\exp\{-L[|\alpha(t)|^2 + |\beta(t)|^2]\}] = 0, \tag{11}$$

where we have evaluated the unitary operator $\hat{T}$ using its normally ordered form

$$\hat{T} =: \prod_{r,s} \exp\left\{\left(e^{\frac{2\pi i}{L}(r+s/n)} - 1\right)\hat{a}^\dagger_{r,s}\hat{a}_{r,s}\right\}: . \tag{12}$$

The polarization is therefore constant in time. Clearly, there is no connection between the net particle transport and the change of the many-body polarization. But it is even more surprising that the latter does not wind irrespective of the path taken in parameter space. We will show in the following that the absence of polarization winding is a generic feature of Gaussian bosonic systems that is in sharp contrast to the fermionic analog.

III. POLARIZATION FOR BOSONS

The goal of this section is to calculate the expectation value of the unitary operator

$$\hat{T} = \exp\left(\frac{2\pi i}{L}\sum_{r,s}\left(r + \frac{s}{n}\right)\hat{a}^\dagger_{r,s}\hat{a}_{r,s}\right). \tag{13}$$

Here $\hat{a}^\dagger_{r,s}$, $\hat{a}_{r,s}$ are bosonic creation and annihilation operators, respectively, where $r = 0, \ldots, L-1$ labels unit cells and $s = 0, \ldots, n-1$ denotes internal sites in the unit cell. $0 \leqslant \frac{s}{n} < 1$ and we have set the lattice constant equal to unity. The results of the following discussion also do not depend on the dimension of the system nor the total number of particles. We note that the operator $\hat{T}$ is not gauge invariant because it changes under an arbitrary shift of the origin of the spatial coordinate system. Throughout this paper, we choose a coordinate system in which $\exp(\frac{2\pi i}{L}(r + \frac{s}{n})) \neq 1$ for any r, s.

We consider a general bosonic Gaussian state [37,38] ρ, which can be formally expressed in diagonal form (Glauber-Sudarshan representation [39,40]) in terms of multimode coherent states,

$$\rho = \int d^2\boldsymbol{\alpha}\, \mathcal{P}(\boldsymbol{\alpha})\, |\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}|, \tag{14}$$

where $d^2\alpha = d\alpha_r d\alpha_i$, with $\alpha_r = (\alpha + \alpha^*)/2$ and $\alpha_i = (\alpha - \alpha^*)/(2i)$ being the real and imaginary parts of the coherent amplitude,

$$\mathcal{P}(\boldsymbol{\alpha}) = \mathcal{N}\int d^2\boldsymbol{\eta}\exp\left(-\frac{1}{2}\boldsymbol{\eta}^T(\mathbf{V} - \mathbb{1})\boldsymbol{\eta} - i(2\boldsymbol{\alpha} + \boldsymbol{\alpha}_0)^T\boldsymbol{\eta}\right). \tag{15}$$

Here $\mathbb{1}$, $\boldsymbol{\alpha} = ((\alpha_{1,r}, \alpha_{1,i}), (\alpha_{2,r}, \alpha_{2,i}), \ldots)$, and $\boldsymbol{\eta} = ((\eta_{1,r}, \eta_{1,i}), (\eta_{2,r}, \eta_{2,i}), \ldots)$ represent the identity matrix and real vectors, respectively, with dimension $2nL$ (note that nL is the number of bosonic modes of the problem). $\mathcal{N}$ is a normalization constant ensuring that $\int d^2\boldsymbol{\alpha}\,\mathcal{P}(\boldsymbol{\alpha}) = 1$. The explicit form of $\mathcal{N}$ is not relevant for our purposes. $\boldsymbol{\alpha}_0 = (\langle\hat{a} + \hat{a}^\dagger\rangle, -i\langle\hat{a} - \hat{a}^\dagger\rangle)^T$ encodes the expectation values of the mode operators, and $\mathbf{V}$ is the $2nL \times 2nL$ covariance matrix of the system, which for a single mode and $n = 1$ reads

$$\mathbf{V} = \begin{pmatrix} \langle\langle\hat{q}\hat{q}\rangle\rangle & \frac{1}{2}\langle\langle\hat{p}\hat{q} + \hat{q}\hat{p}\rangle\rangle \\ \frac{1}{2}\langle\langle\hat{p}\hat{q} + \hat{q}\hat{p}\rangle\rangle & \langle\langle\hat{p}\hat{p}\rangle\rangle \end{pmatrix}. \tag{16}$$

Here $\hat{q} = \hat{a} + \hat{a}^\dagger$ and $\hat{p} = -i(\hat{a} - \hat{a}^\dagger)$, and $\langle\langle xy\rangle\rangle = \langle xy\rangle - \langle x\rangle\langle y\rangle$. $\mathbf{V}$ is a real and symmetric matrix by construction and is also positive-definite due to the Heisenberg uncertainty principle. $\mathcal{P}$ is positive and well defined if furthermore $\mathbf{V} > \mathbb{1}$. In this case, the state is a statistical mixture of coherent states, i.e., a classical state. A quantum state is considered to be nonclassical if it cannot be written as a statistical mixture of coherent states. In this paper, we consider more general bosonic Gaussian states. (A good introduction to bosonic Gaussian states can be found, for example, in [37].)

$\mathcal{P}(\boldsymbol{\alpha})$ can be used to evaluate the expectation value of any normally ordered operator function $:f(\{\hat{a}^\dagger_\mu, \hat{a}_\mu\}):$ by the replacement $(\hat{a}^\dagger \to \alpha^*)$ and $(\hat{a} \to \alpha)$ and integration. The $\mathcal{P}$ function may be singular and can attain negative values. All integration with $\mathcal{P}(\boldsymbol{\alpha})$ must therefore be understood in the distributional sense.

Using Eq. (12), we find

$$\langle\hat{T}\rangle = \mathcal{N}_1\int d^2\boldsymbol{\eta}\int d^2\boldsymbol{\alpha}\exp\left\{-\frac{1}{2}\boldsymbol{\eta}^T(\mathbf{V} - 11)\boldsymbol{\eta} - i\boldsymbol{\alpha}_0^T\boldsymbol{\eta}\right\} \times \exp\{-2i\boldsymbol{\alpha}\boldsymbol{\eta}^T - \boldsymbol{\alpha}^T(\mathbb{1} - \mathbf{U})\boldsymbol{\alpha}\}, \tag{17}$$

where $\mathbf{U}$ is a unitary operator

$$(\mathbf{U})_{r_1,s_1;r_2,s_2} = \exp\left(\frac{2\pi i}{L}\left(r_1 + \frac{s_1}{n}\right)\right)\delta_{r_1 r_2}\delta_{s_1,s_2}. \tag{18}$$

According to our assumption $[\exp(\frac{2\pi i}{L}(r+\frac{s}{n})) \neq 1]$, $\mathbb{1}-\mathbf{U}$ is an invertible symmetric complex matrix. In addition, its real part $\mathbb{1}-\frac{\mathbf{U}+\mathbf{U}^\dagger}{2}$ is positive-definite. In this case, the Gaussian integral (17) over $\boldsymbol{\alpha}$ is well-defined and is proportional to $[\det(\mathbb{1}-\mathbf{U})]^{-1/2}$. We note that when the matrix is complex, the calculation of the square root requires some special care. However, one can show that any symmetric complex matrix has a unique symmetric square root whose real part is positive-definite [41]. After successive integration over $\boldsymbol{\alpha}$ and then over $\boldsymbol{\eta}$ we eventually obtain

$$\langle \hat{T} \rangle = \mathcal{N}_2\left[\det(\mathbf{V}+\mathbb{1})\det\left(\mathbb{1} - \frac{\mathbf{V}-\mathbb{1}}{\mathbf{V}+\mathbb{1}}\mathbf{U}\right)\right]^{-1/2} \times \exp\left(-\frac{1}{2}\boldsymbol{\alpha}_0^T\mathbf{M}^{-1}\boldsymbol{\alpha}_0\right), \tag{19}$$

where $\mathcal{N}_2 = 2^{nL}$ and

$$\mathbf{M} = \mathbf{V} - \mathbb{1} + 2(\mathbb{1}-\mathbf{U})^{-1}. \tag{20}$$

Substituting this expectation value into the expression of the many-body polarization (1), one obtains

$$\begin{aligned} P &= -\frac{1}{4\pi}\mathrm{Im}\ln\left[\det(\mathbf{V}+\mathbb{1})\det\left(\mathbb{1}-\frac{\mathbf{V}-\mathbb{1}}{\mathbf{V}+\mathbb{1}}\mathbf{U}\right)\right] \\ &\quad - \frac{1}{4\pi}\mathrm{Im}\left(-\frac{1}{2}\boldsymbol{\alpha}_0^T\mathbf{M}^{-1}\boldsymbol{\alpha}_0\right) \\ &= -\frac{1}{4\pi}\mathrm{Im}\ln[\det(\mathbb{1}-\mathbf{W})] - \frac{1}{4\pi}\mathrm{Im}\left(-\frac{1}{2}\boldsymbol{\alpha}_0^T\mathbf{M}^{-1}\boldsymbol{\alpha}_0\right), \end{aligned} \tag{21}$$

where

$$\mathbf{W} = \frac{\mathbf{V}-\mathbb{1}}{\mathbf{V}+\mathbb{1}}\mathbf{U}. \tag{22}$$

One can show that the second term in Eq. (21) is a single-valued function of system parameters and therefore does not contribute to the change of polarization. In the next section, we will show that the first term in Eq. (21) vanishes in the thermodynamic limit of infinite system size $L \to \infty$.

IV. POLARIZATION IN THE THERMODYNAMIC LIMIT

A. Polarization scaling: Bosons versus fermions

In Ref. [18] it was shown that the polarization of a general Gaussian mixed state ρ of lattice fermions at commensurate filling can be written as a sum of the polarization of a pure state $|\psi\rangle$ plus a term that vanishes in the thermodynamic limit of infinite system size $L \to \infty$,

$$P(\rho) = P(|\psi\rangle\langle\psi|) + O(L^{-\alpha}), \quad \alpha > 0. \tag{23}$$

Here $|\psi\rangle$ is the many-body ground state of the so-called fictitious Hamiltonian. In the following, we will assume that the second term in Eq. (21) vanishes, and we show that the remaining term in the bosonic case yields

$$P(\rho) = 0 + O(e^{-\alpha L}), \quad \alpha > 0. \tag{24}$$

For the sake of simplicity, we restrict ourselves to the simplest nontrivial case of a two-band model, e.g., resulting from a tight-binding Hamiltonian with a unit cell of two lattice sites. The generalization to the case of multiple bands is, however, straightforward.

We introduce the Fourier transform given by the unitary block matrix $\mathbf{U}_{\mathrm{FT}}$,

$$(\mathbf{U}_{\mathrm{FT}})_{jk} \equiv \frac{1}{\sqrt{L}}\exp\left(\frac{2\pi i}{L}jk\right)\mathbb{1}_4. \tag{25}$$

As a consequence of the periodic boundary conditions, the covariance matrix $\mathbf{V}$ is block-circulant. Since the model has lattice translational invariance, the covariance matrix is diagonalized by the Fourier transform, and we can write

$$\mathbf{U}_{\mathrm{FT}}\frac{\mathbf{V}-\mathbb{1}_{4L}}{\mathbf{V}+\mathbb{1}_{4L}}\mathbf{U}_{\mathrm{FT}}^\dagger = \bigoplus_{k=0}^{L-1}\frac{\mathbf{v_k}-\mathbb{1}_4}{\mathbf{v_k}+\mathbb{1}_4}, \tag{26}$$

where $\oplus$ denotes the direct sum, which constructs a block-diagonal matrix. The transformed unitary matrix $\mathbf{U}$, given by Eq. (18), is

$$(\mathbf{U}_{\mathrm{FT}}\,\mathbf{U}\,\mathbf{U}_{\mathrm{FT}}^\dagger)_{j,s_1;k,s_2} = \delta_{j,k+1}\delta_{s_1 s_2}\exp\left(\frac{2\pi i}{L}\frac{s_1}{n}\right)\mathbb{1}_4. \tag{27}$$

To make the following expressions more compact, we furthermore introduce $\mathbf{m}_k \equiv \frac{\mathbf{v_k}-\mathbb{1}_4}{\mathbf{v_k}+\mathbb{1}_4}[\mathbb{1}_2 \oplus \exp(\frac{i\pi}{L})\mathbb{1}_2]$. The determinant in Eq. (21) can thus be written as

$$\det\left(\mathbb{1}-\frac{\mathbf{V}-\mathbb{1}}{\mathbf{V}+\mathbb{1}}\mathbf{U}\right) = \begin{vmatrix} \mathbb{1}_4 & 0 & & & & -\mathbf{m}_{L-1} \\ -\mathbf{m}_0 & \mathbb{1}_4 & 0 & & & \\ 0 & -\mathbf{m}_1 & \mathbb{1}_4 & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & -\mathbf{m}_{L-3} & \mathbb{1}_4 & 0 \\ 0 & & & 0 & -\mathbf{m}_{L-2} & \mathbb{1}_4 \end{vmatrix}. \tag{28}$$

This block determinant can be reduced by applying Schur's identity iteratively. This yields a determinant of dimension 4×4:

$$\det\left(\mathbb{1}-\frac{\mathbf{V}-\mathbb{1}}{\mathbf{V}+\mathbb{1}}\mathbf{U}\right) = \det\left(\mathbb{1}_4 - \prod_{k=0}^{L-1}\mathbf{m}_k\right). \tag{29}$$

We note that up to this point there is a formal analogy of the polarization for Gaussian states of bosons and that of fermions, as discussed in Ref. [18]. There the matrices $\mathbf{m}_k \sim e^{-B_k}U_{k+1}^\dagger U_k$ contained unitary matrices U_k and weighting factors $e^{-B_k} = \mathrm{diag}_s(e^{-\beta_{k,s}})$. To be specific, let us consider a grand-canonical thermal state of a fermionic insulator with a chemical potential μ within a band gap. Then all bands s with energies below μ lead to a negative exponent $\beta_{k,s} = \beta(\epsilon_{k,s}-\mu)$ and thus to weighting factors bigger than unity. This results in an amplification of contributions from occupied bands, which is the essence of the gauge-reduction mechanism for Gaussian states of fermions found in [18].

The situation is completely different, however, in the case of bosons. Since the covariance matrix $\mathbf{V}$ of Gaussian states of bosons is positive-definite, the resulting k-dependent 4×4 blocks have eigenvalues $\lambda(\mathbf{m}_k)$ with absolute values obeying

$$|\lambda(\mathbf{m}_k)| < 1, \qquad \forall\, k = 0, \dots, L-1. \tag{30}$$

We define the corresponding maximum absolute eigenvalue:

$$\lambda_{\max} \equiv \max_i \left| \lambda_i \left(\frac{\mathbf{V} - \mathbb{1}}{\mathbf{V} + \mathbb{1}} \right) \right|. \tag{31}$$

According to Eq. (31), a single matrix $\mathbf{m}_k$ is bounded and thus the product of matrices must be bounded as well, i.e., $\| \prod_k \mathbf{m}_k \| = O((\lambda_{\max})^L)$. If $\lambda_{\max} = 0$, the polarization vanishes trivially, otherwise we split off the maximum absolute eigenvalues $\mathbf{A} \equiv (\lambda_{\max})^{-L} \prod_k \mathbf{m}_k$ such that $|\mathrm{Tr}(\mathbf{A})| \leqslant 4$ and we define a small parameter $\epsilon \equiv 4(\lambda_{\max})^L$. We can then express the polarization P by expanding the determinant and logarithm in this small parameter:

$$\begin{aligned} \ln\det\left(\mathbb{1}_4 - \prod_k \mathbf{m}_k\right) &= \ln\det\left(\mathbb{1}_4 - \frac{\epsilon}{4}\mathbf{A}\right) \\ &= \ln\left(1 - \frac{\epsilon}{4}\mathrm{Tr}(\mathbf{A}) + O(\epsilon^2)\right) \\ &= -\frac{\epsilon}{4}\mathrm{Tr}(\mathbf{A}) + O(\epsilon^2). \end{aligned} \tag{32}$$

With this we find the following system-size scaling of the polarization for Gaussian bosonic states:

$$\begin{aligned} 4\pi|P| &\leqslant \frac{\epsilon}{4}|\mathrm{Tr}(\mathbf{A})| + O(\epsilon^2) \\ &\leqslant \epsilon + O(\epsilon^2). \end{aligned} \tag{33}$$

Since we know that $0 \leqslant \lambda_{\max} < 1$, the small parameter ϵ vanishes exponentially in L,

$$\alpha \equiv -\ln(\lambda_{\max}) > 0 \Rightarrow \epsilon = 4e^{-\alpha L}.$$

Therefore, as the system approaches the thermodynamic limit, the first term of the many-body polarization in Eq. (21) vanishes exponentially and only the trivial second term remains. For equilibrium states at finite T this has a simple physical interpretation: The chemical potential for (noninteracting) bosons is always less than the smallest single-particle energy. As a consequence, *all* weighting factors $e^{-\beta_{k,s}}$ are strictly less than unity and there is no amplification that leads to a gauge reduction as in the case of fermions. Thus the absence of the Pauli exclusion principle for (noninteracting) bosons also leads to the absence of a gauge reduction mechanism as in Ref. [18].

As an illustration of our results, we analyze the bosonic Rice-Mele model with the initial state (7). The covariance matrix of this state is just the identity [37], and therefore, as was expected, the expression of P [Eq. (21)] coincides with Eq. (11).

B. Polarization amplitude

Since the many-body polarization is defined as the complex phase of the lattice momentum shift, it can only be defined if the absolute value $|\langle \hat{T} \rangle|$ does not vanish throughout the entire adiabatic evolution. It turns out that this is always true for finite system sizes. However, as noted by Resta and Sorella, $|\langle \hat{T} \rangle|$ is a measure for the localization of single-particle states [29], which in the thermodynamic limit approaches unity for an insulator and vanishes for a conductor. Thus for noninteracting bosons we expect it to decay when $L \to \infty$. Both can be seen by inserting Eq. (29) into Eq. (19) and taking the absolute value:

$$\begin{aligned} |\langle \hat{T} \rangle| = {} & 2^{nL} |\det(\mathbb{1}_{2nL} + \mathbf{V})|^{-1/2} \\ & \times \left| \det\left(\mathbb{1}_{2n} - \prod_{k=0}^{L-1} \mathbf{m}_k\right) \right|^{-1/2} \left| \exp\left(-\frac{1}{2}\boldsymbol{\alpha}_0^T \mathbf{M}^{-1} \boldsymbol{\alpha}_0\right) \right|. \end{aligned} \tag{34}$$

We proceed by finding upper and lower bounds. To this end, we note that for the absolute value of the last exponential term only the Hermitian part of the matrix contributes $\frac{1}{2}(\mathbf{M} + \mathbf{M}^\dagger) = \mathbf{V}$. Thus

$$0 < \left| \exp\left(-\tfrac{1}{2}\boldsymbol{\alpha}_0^T \mathbf{M}^{-1} \boldsymbol{\alpha}_0\right) \right| < 1. \tag{35}$$

From this one can see that $|\langle \hat{T} \rangle|$ is always positive for finite system sizes L. Denoting the minimum eigenvalue of $\mathbf{V}$ by $\lambda_{\min}^{\mathrm{V}}$ and assuming a classical state, i.e., $\lambda_{\min}^{\mathrm{V}} > 1$, one can derive an upper bound that scales in the system size nL:

$$0 < |\langle \hat{T} \rangle| < \left(\frac{1 + \lambda_{\min}^{\mathrm{V}}}{2} \right)^{-nL} < 1. \tag{36}$$

From this we can see that the many-body polarization P is well-defined for all system sizes $L < \infty$ and that classical states exhibit negligible single-particle localization for large L.

V. POLARIZATION WINDING

In one-dimensional lattice systems with a Hamiltonian or a Liouvillian, which depend on an external parameter λ in a cyclic way, the winding of the EGP or the many-body polarization with λ defines a topological invariant:

$$w = \Delta P = \oint d\lambda \frac{\partial P(\lambda)}{\partial \lambda}. \tag{37}$$

In two-dimensional translationally invariant lattice models, a similar construction defines a Chern number. For example, introducing particle number operators in mixed real and momentum space by performing a discrete Fourier transformation in one direction (e.g., y), $\hat{a}_j(k_y) \sim \sum_l \hat{a}_{j,l} \exp(2\pi i l k_y/L)$, one can define a momentum-dependent polarization (where we have suppressed band indices for simplicity)

$$P_x(k_y) = \frac{1}{2\pi} \mathrm{Im} \ln \left\langle \exp\left(\frac{2\pi i}{L} \sum_j j \hat{a}_j^\dagger(k_y) \hat{a}_j(k_y) \right) \right\rangle. \tag{38}$$

The winding of $P(k)$ when going through the Brillouin zone in k defines a Chern number,

$$C = \int_{\mathrm{BZ}} dk_y \frac{\partial P_x(k_y)}{\partial k_y} = \int_{\mathrm{BZ}} dk_x \frac{\partial P_y(k_x)}{\partial k_x}. \tag{39}$$

If we consider the polarization in a Gaussian mixed state of bosons $\rho(\lambda)$, which is uniquely defined along a closed path of the parameter λ in parameter space, we can argue from Eq. (24) that the winding of the many-body polarization vanishes for a sufficiently large but finite system size L. This is because of the exponential bound that yields $-\frac{1}{2} < P < +\frac{1}{2}$ if the system is large enough. As a consequence, all many-body topological invariants based on the winding of the polarization are trivial for sufficiently large systems. In the following, we will explicitly show that this holds true independently of the system size.

Let us assume that the polarization is a function of two real parameters that change cyclically in time from 0 to T. Then the change of the polarization between times $t = 0$ and $t = T$ can be described as a loop along a closed path $\mathcal{C}$ in parametric space. The two parameters can be combined into a complex variable χ. Thus the change of polarization can be written as

$$\Delta P = -\frac{1}{4\pi}\,\mathrm{Im}\oint_{\mathcal{C}} d\chi \frac{\partial}{\partial\chi}\ln\det[\mathbb{1}_{2nL} - \mathbf{W}(\chi)]. \tag{40}$$

Moreover, using

$$\frac{\partial}{\partial\chi}\ln\det[\mathbb{1} - \mathbf{W}(\chi)] = \mathrm{Tr}\left[[\mathbb{1} - \mathbf{W}(\chi)]^{-1}\frac{\partial(\mathbb{1} - \mathbf{W}(\chi))}{\partial\chi}\right] \tag{41}$$

we derive the following expression for ΔP:

$$\Delta P = \frac{1}{4\pi}\,\mathrm{Im}\,\mathrm{Tr}\oint_{\mathcal{C}} d\chi\left[[\mathbb{1} - \mathbf{W}(\chi)]^{-1}\frac{\partial(\mathbb{1} - \mathbf{W}(\chi))}{\partial\chi}\right]. \tag{42}$$

The expression (41) can be derived from the identity $\ln(\det(A(z))) = \mathrm{Tr}(\ln A(z))$ [for a rigorous derivation of (41), the reader is referred to [42]].

Now we are ready to prove that the change of polarization vanishes for any bosonic Gaussian state. For that we first review some facts about zeros of determinants of holomorphic matrix-valued functions (for more details, see [43]).

Let $\mathbf{F}(\chi)$ be a matrix-valued function that is analytic in a domain C. Under the assumption that all values of $\mathbf{F}(\chi)$ on the boundary $\mathcal{C}$ of C are invertible operators, it is possible to show [43] that

$$\mathcal{M} = \frac{1}{2\pi i}\mathrm{Tr}\oint_{\mathcal{C}} d\chi\left[\mathbf{F}(\chi)^{-1}\frac{d\mathbf{F}(\chi)}{d\chi}\right]$$

is the number of zeros of $\det\mathbf{F}(\chi)$ inside $\mathcal{C}$ (including their multiplicities). Combining this with Eq. (42), we obtain

$$\Delta P = \tfrac{1}{2}\mathcal{M}, \tag{43}$$

where $\mathcal{M}$ is the number of solutions (zeros) of

$$\det[\mathbb{1} - \mathbf{W}(\chi)] = 0$$

inside the closed path $\mathcal{C}$ in parametric space. To estimate $\mathcal{M}$, we use a generalization of Rouché's theorem for the matrix valued complex function [43], which states the following:

Rouché's theorem: Let $\mathcal{C}$ be a closed contour bounding a domain C. If $\|\mathbf{F}(\chi)\| < 1$ on $\mathcal{C}$, then

$$\frac{1}{2\pi i}\mathrm{Tr}\oint_{\mathcal{C}} d\chi\left[[\mathbb{1}+\mathbf{F}(\chi)]^{-1}\frac{d\mathbf{F}(\chi)}{d\chi}\right] = 0.$$

Applying Rouché's theorem to our problem, where

$$\|\mathbf{F}(\chi)\| = \|\mathbf{W}(\chi)\| = \left\|\frac{\mathbf{V} - \mathbb{1}}{\mathbf{V} + \mathbb{1}}\right\| < 1,$$

we see that for any $\mathbf{V} > 0$, i.e., for any Gaussian bosonic state,

$$\|\mathbf{W}(\chi)\| < 1.$$

Therefore, the change of polarization is equal to zero, irrespective of the system size,

$$\Delta P = 0. \tag{44}$$

We note that this result is again a direct consequence of the positivity of the covariance matrix $\mathbf{V}$ for Gaussian states of *bosons*. This proves that for any bosonic Gaussian state, the total change of the many-body polarization along a closed path in parametric space is zero. This is in sharp contrast to free fermion systems in which the winding of the many-body polarization is a topologically quantized observable and can be nontrivial.

VI. CONCLUSION

We have shown that the many-body polarization of translationally invariant Gaussian states of bosons approaches zero in the thermodynamic limit of infinite system size. Its winding upon a cyclic change of the state, which in the case of fermions defines a many-body topological invariant, vanishes for any system size. Thus many-body topological invariants based on the polarization are always trivial in finite-temperature states or Gaussian nonequilibrium states of noninteracting bosons. This is also the case if the band structure of the underlying lattice Hamiltonian is topologically nontrivial, i.e., it possesses bands with a nonvanishing Chern number. As a consequence, there is no topologically protected quantized charge transport of Gaussian states of bosons, and the latter requires strong interactions [44]. This property of bosons is in sharp contrast to fermions, which can be topologically nontrivial even in many-body states that are not gapped, such as high-temperature states of band insulators, and is a consequence of the absence of a Pauli exclusion principle.

ACKNOWLEDGMENT

Financial support from the DFG (Project No. 277625399) through SFB TR 185 is gratefully acknowledged.

[1] Y. Hatsugai, Chern Number and Edge States in the Integer Quantum Hall Effect, Phys. Rev. Lett. **71**, 3697 (1993).

[2] K. V. Klitzing, G. Dorda, and M. Pepper, New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance, Phys. Rev. Lett. **45**, 494 (1980).

[3] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Quantized Hall Conductance in a Two-Dimensional Periodic Potential, Phys. Rev. Lett. **49**, 405 (1982).

[4] D. J. Thouless, Quantization of particle transport, Phys. Rev. B **27**, 6083 (1983).

[5] Q. Niu and D. J. Thouless, Quantised adiabatic charge transport in the presence of substrate disorder and many-body interactions, J. Phys. A **17**, 2453 (1984).

[6] S. Nakajima, T. Tomita, S. Taie, T. Ichinose, H. Ozawa, L. Wang, M. Troyer, and Y. Takahashi, Topological Thouless pumping of ultracold fermions, Nat. Phys. **12**, 296 (2016).

[7] D. C. Tsui, H. L. Störmer, and A. C. Gossard, Two-Dimensional Magnetotransport in the Extreme Quantum Limit, Phys. Rev. Lett. **48**, 1559 (1982).

[8] R. B. Laughlin, Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations, Phys. Rev. Lett. **50**, 1395 (1983).

[9] D. Arovas, J. R. Schrieffer, and F. Wilczek, Fractional Statistics and the Quantum Hall Effect, Phys. Rev. Lett. **53**, 722 (1984).

[10] C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. Das Sarma, Non-Abelian anyons and topological quantum computation, Rev. Mod. Phys. **80**, 1083 (2008).

[11] J. E. Avron, M. Fraas, G. M. Graf, and O. Kenneth, Quantum response of dephasing open systems, New J. Phys. **13**, 053042 (2011).

[12] C.-E. Bardyn, M. A. Baranov, C. V. Kraus, E. Rico, A. Imamoglu, P. Zoller, and S. Diehl, Topology by dissipation, New J. Phys. **15**, 085001 (2013).

[13] O. Viyuela, A. Rivas, and M. A. Martin-Delgado, Uhlmann Phase as a Topological Measure for One-Dimensional Fermion Systems, Phys. Rev. Lett. **112**, 130401 (2014).

[14] O. Viyuela, A. Rivas, and M. A. Martin-Delgado, Two-Dimensional Density-Matrix Topological Fermionic Phases: Topological Uhlmann Numbers, Phys. Rev. Lett. **113**, 076408 (2014).

[15] Z. Huang and D. P. Arovas, Topological Indices for Open and Thermal Systems Via Uhlmann's Phase, Phys. Rev. Lett. **113**, 076407 (2014).

[16] E. P. L. van Nieuwenburg and S. D. Huber, Classification of mixed-state topology in one dimension, Phys. Rev. B **90**, 075141 (2014).

[17] D. Linzner, L. Wawer, F. Grusdt, and M. Fleischhauer, Reservoir-induced Thouless pumping and symmetry protected topological order in open quantum chains, Phys. Rev. B **94**, 201105(R) (2016).

[18] C. E. Bardyn, L. Wawer, A. Altland, M. Fleischhauer, and S. Diehl, Probing the Topology of Density Matrices, Phys. Rev. X **8**, 011035 (2018).

[19] M. V. Berry, Quantal phase factors accompanying adiabatic changes, Proc. R. Soc. A **392**, 45 (1984).

[20] F. Wilczek and A. Zee, Appearance of Gauge Structure in Simple Dynamical Systems, Phys. Rev. Lett. **52**, 2111 (1984).

[21] J. Zak, Berry's Phase for Energy Bands in Solids, Phys. Rev. Lett. **62**, 2747 (1989).

[22] D. Xiao, M. C. Chang, and Q. Niu, Berry phase effects on electronic properties, Rev. Mod. Phys. **82**, 1959 (2010).

[23] M. J. Rice and E. J. Mele, Elementary Excitations of a Linearly Conjugated Diatomic Polymer, Phys. Rev. Lett. **49**, 1455 (1982).

[24] L. Wang, M. Troyer, and X. Dai, Topological Charge Pumping in a One-Dimensional Optical Lattice, Phys. Rev. Lett. **111**, 026802 (2013).

[25] A. Uhlmann, Parallel transport and "quantum holonomy" along density operators, Rep. Math. Phys. **24**, 229 (1986).

[26] J. C. Budich and S. Diehl, Topology of density matrices, Phys. Rev. B **91**, 165140 (2015).

[27] R. Resta, Quantum Mechanical Position Operator in Extended Systems, Phys. Rev. Lett. **80**, 1800 (1998).

[28] R. D. King-Smith and D. Vanderbilt, Theory of polarization of crystalline solids, Phys. Rev. B **47**, 1651 (1993).

[29] R. Resta and S. Sorella, Electron Localization in the Insulating State, Phys. Rev. Lett. **82**, 370 (1999).

[30] A. A. Aligia and G. Ortiz, Quantum Mechanical Position Operator and Localization in Extended Systems, Phys. Rev. Lett. **82**, 2560 (1999).

[31] M. Nakamura and J. Voit, Lattice twist operators and vertex operators in sine-Gordon theory in one dimension, Phys. Rev. B **65**, 153110 (2002).

[32] R. Kobayashi, Y. O. Nakagawa, Y. Fukusumi, and M. Oshikawa, Scaling of the polarization amplitude in quantum many-body systems in one dimension, Phys. Rev. B **97**, 165133 (2018).

[33] A. Altland, and M. R. Zirnbauer, Nonstandard symmetry classes in mesoscopic normal-superconducting hybrid structures, Phys. Rev. B **55**, 1142 (1997).

[34] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Classification of topological insulators and superconductors in three spatial dimensions, Phys. Rev. B **78**, 195125 (2008).

[35] S. Ryu, A. P. Schnyder, A. Furusaki, and A. W. W. Ludwig, Topological insulators and superconductors: Ten-fold way and dimensional hierarchy, New J. Phys. **12**, 7 (2010).

[36] L. Wawer, R. Li, and M. Fleischhauer (unpublished).

[37] Ch. Weedbrook, S. Pirandola, R. Garcia-Patron, N. J. Cerf, T. C. Ralph, J. H. Shapiro, and S. Lloyd, Gaussian quantum information, Rev. Mod. Phys. **84**, 621 (2012).

[38] A. S. Holevo, M. Sohma, and O. Hirota, Capacity of quantum Gaussian channels, Phys. Rev. A **59**, 1820 (1999).

[39] E. C. G. Sudarshan, Equivalence of Semiclassical and Quantum Mechanical Descriptions of Statistical Light Beams, Phys. Rev. Lett. **10**, 277 (1963).

[40] R. J. Glauber, The quantum theory of optical coherence, Phys. Rev. **130**, 2529 (1963).

[41] T. Kato, *Perturbation Theory for Linear Operators* (Springer, Berlin, Heidelberg, 1995).

[42] C. Gohberg and M. G. Krein, *Introduction to the Theory of Linear Nonselfadjoint Operators in Hilbert Space*, Math. Monographs Vol. 18 (American Mathematical Society, Providence, RI, 1969), p. 163.

[43] I. Gohberg, S. Goldberg, and M. A. Kaashoek, *Classes of Linear Operators*, Vol. I, Operator Theory: Advances and Applications Vol. 49 (Birkhäuser, Basel, 1990).

[44] M. Lohse, C. Schweizer, O. Zilberberg, M. Aidelsburger, and I. Bloch, A Thouless quantum pump with ultracold bosonic atoms in an optical superlattice, Nat. Phys. **12**, 350 (2015).