

Geometric phases and quantum entanglement as building blocks for non-Abelian quasiparticle statistics

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Some models describing unconventional fractional quantum Hall states predict quasiparticles that obey non-Abelian quantum statistics. The most prominent example is the Moore-Read model for the $\nu=5/2$ state, in which the ground state is a superconductor of composite fermions, the charged excitations are vortices in that superconductor, and the non-Abelian statistics is closely linked to the degeneracy of the ground state in the presence of vortices. In this paper we develop a physical picture of the non-Abelian statistics of these vortices. Considering first the positions of the vortices as fixed, we define a set of single-particle states at and near the core of each vortex, and employ general properties of the corresponding Bogolubov-de Gennes equations to write the ground states in the Fock space defined by these single-particle states. We find all ground states to be *entangled superpositions* of all possible occupations of the single-particle states near the vortex cores, in which the probability for all occupations is equal, and the relative phases vary from one ground state to another. Then, we examine the evolution of the ground states as the positions of the vortices are braided. We find that as vortices move, they accumulate a *geometric phase* that depends on the occupations of the single-particle states near the cores of other vortices. Thus, braiding of vortices changes the relative phase between different components of a superposition, in which the occupations of these states differ, and hence transform the system from one ground state to another. These transformations, that emanate from the quantum entanglement of the occupations of single-particle states and from the dependence of the geometric phase on these occupations, are the source of the non-Abelian statistics. Finally, by exploring a “self-similar” form of the many-body wave functions of the various ground states, we show the equivalence of our picture, in which vortex braiding leads to a change in the relative phase of components in a superposition, and pictures derived previously, in which vortex braiding seemingly affects the occupations of states in the cores of the vortices.

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I. INTRODUCTION

The experimental discovery¹ of the fractional quantum Hall effect (FQHE) led to intriguing theoretical observations regarding the elementary excitations (quasiparticles) of a two-dimensional electron system at a fractional Landau-level filling factor ν . Very soon after the experimental discovery, Laughlin² realized that the quasiparticles at filling factors $\nu = 1/(2p+1)$ (with p an integer) carry a fractional charge $e^* = \pm e/(2p+1)$ (for brevity, we use the term quasiparticles to refer also to quasiholes). Following that observation, Halperin³ showed that the hierarchy of observed FQHE states, at $\nu=p/q$ (with q an odd integer), points to the fractional statistics of the quasiparticles and quasiholes, of the type that was previously studied by Wilczek.⁴ This observation was further clarified by Arovas, Schrieffer, and Wilczek.⁵ When a system contains two quasiparticles, and the positions of these quasiparticles are adiabatically interchanged, the state of the system acquires a geometric Berry

phase. This phase, which is π for fermions and 2π for bosons, becomes a fraction of π for FQHE quasiparticles.

The experimental discovery⁶ of the even-denominator FQHE state $\nu=5/2$ triggered the introduction of yet another novel concept with regard to the statistics of the elementary excitations. Employing conformal field theory to study the $\nu=5/2$ FQHE, Moore and Read⁷ discovered that if this state is well described by the Pfaffian wave function, as numerical investigations seem to confirm,⁸ the elementary excitations obey non-Abelian statistics. The state of the system after a series of quasiparticle interchanges then depends on the order in which these interchanges are carried out. By using exact eigenstates of a model Hamiltonian,⁹ Nayak and Wilczek¹⁰ subsequently showed that the ground state of the configuration in which $2N$ quasiholes are inserted at fixed positions is 2^N -fold degenerate, and that the quasiparticles realize a 2^{N-1} -dimensional spinor braiding statistics. Effective Chern-Simons theories and their relations to non-Abelian statistics have been studied in Ref. 11.

Following earlier observations that related the Pfaffian state to p -wave Cooper pairing, Read and Green¹² described this state as a p -wave BCS superconductor of composite fermions, and conjectured that the non-Abelian statistics of its quasiparticles results from the zero-energy modes associated with vortices in this superconductor. This conjecture was further studied by Ivanov,¹³ who mapped out the relation between the exchange of quasiparticles and the unitary transformation carried out on the Hilbert space of the ground states. Ivanov explicitly derived these unitary transformations, showed that they are indeed non-Abelian, and confirmed that they are identical to the transformations derived earlier by Nayak and Wilczek¹⁰ using conformal field theory.

While these two derivations of the unitary transformations associated with vortex interchange may be easily generalized to calculate the transformations associated with other braidings of vortices, they do not provide a clear physical picture of the non-Abelian statistics. This is exemplified in the following observation: using the method of Ref. 13, it is easy to show that when the system is initially in a ground state $|g.s._\alpha\rangle$, and vortex j encircles vortex $j+1$, then, under the assumption that no tunneling takes place between the vortex cores, the final state of the system is again a ground state, given by

$$(c_j e^{(i/2)\Omega_j} + c_j^\dagger e^{-(i/2)\Omega_j})(c_{j+1} e^{(i/2)\Omega_{j+1}} + c_{j+1}^\dagger e^{-(i/2)\Omega_{j+1}})|g.s._\alpha\rangle, \quad (1)$$

where the operators $c_j^{(\dagger)}$, $c_{j+1}^{(\dagger)}$ annihilate (create) a particle localized very close to the cores of the j th and $(j+1)$ th vortex, respectively, and Ω_j is a phase defined in the next section. Equation (1) seemingly implies that the motion of the j th vortex around the $(j+1)$ th vortex affects the occupations of states very close to the cores of the two vortices. This is in contrast, however, to the derivation leading to Eq. (1), which explicitly assumes that vortices are kept far enough from one another so that tunneling between vortex cores may be disregarded.

In this work we study the manifold of degenerate ground states $|g.s._\alpha\rangle$ in an attempt to give a physical picture of the effect of braidings in the positions of vortices. We use a second quantized formalism to write these states as many-body wave functions in a carefully defined Fock space, with the positions \mathbf{R}_i of the vortices being parameters in these wave functions. Then, when the vortices are adiabatically moved and these parameters change, the wave functions change, in principle, in two ways: first, through their explicit non-single valued dependence on \mathbf{R}_i , and second, through the induced non-Abelian geometric vector potential matrix, whose matrix elements are $\text{Im}\langle g.s._\alpha | \nabla_{\mathbf{R}_i} | g.s._\alpha \rangle$. We construct the Fock space in such a way that the second contribution vanishes, and the entire time evolution of the wave functions is through their multivalued dependence on the changing coordinates \mathbf{R}_i . Consequently, the unitary transformations associated with the braiding of vortex positions can be read off from the explicit form of the wave functions.

Following our derivation of the ground states we show that two ingredients are essential for the non-Abelian statistics of the vortices. The first is the quantum entanglement of

the occupation of states near the cores of distant vortices. The second ingredient is familiar from (Abelian) fractional statistics: the geometric phase accumulated by a vortex traversing a closed loop.

Within the Chern-Simons composite-boson theory,¹⁴ the Abelian fractional statistics of the $\nu=1/m$ states is explained by mapping the ground state of the electronic system to a superfluid of composite bosons, and the quasiparticle excitations to vortices in that superfluid. Due to the coupling of the vortex to a Chern-Simons gauge field, the depletion of bosons at the vortex core is quantized to a fraction $1/m$ of a fluid particle. Thus the charge carried by the vortex is also fractional. The quantum statistics is related to the geometric phase accumulated by a vortex traversing a close trajectory. Roughly speaking, the vortex accumulates a phase of 2π per fluid particle which it encircles. When another vortex with its fractional charge is introduced to the encircled area, this phase changes by a fraction of 2π . Upon adapting the argument to interchanging of vortices, one finds that this fraction of 2π translates into fractional statistics.

Similarly, the Moore-Read theory of the $\nu=5/2$ state describes it also as a superfluid, with the quasiparticles being vortices in that superfluid. However, the “effective bosons” forming the superfluid are Cooper pairs of composite fermions. Consequently, the superfluid has excitation modes associated with the breaking of Cooper pairs. In the presence of vortices, a Cooper pair may be broken such that one or two of its constituents are localized in the cores of vortices. For p -wave superconductors, the existence of zero-energy intra-vortex modes leads, first, to a multitude of ground states and, second, to a particle-hole symmetric occupation of the vortex cores in all ground states. When represented in occupation-number basis, a ground state is a superposition which has equal probability for the vortex core to be empty or occupied by one fermion.

When a vortex traverses a trajectory that encircles another vortex, the phase it accumulates depends again on the number of fluid particles which it encircles. Since a fluid particle is, in this case, a Cooper pair, the occupation of a vortex core by a fermion, half a pair, leads to an accumulation of a phase of π relative to the case when the core is empty. And since the ground state is a superposition with equal weights for the two possibilities, the relative phase of π introduced by the encircling might in this case transform the system from one ground state to another.

This qualitative picture is made more precise in this paper. Our analysis revolves around the definition of a set of single-particle states localized at or near the $2N$ vortex cores. We start by defining the “core states,” a set of $2N$ states each of which is localized at a specific vortex core. We find that in all possible ground states, the occupation of these single-particle states near one vortex is entangled with the occupation of single-particle states near all other vortices. We prove that any many-body state in which these occupations are disentangled is necessarily an excited state. We show that the evolution of the ground state as positions of vortices are braided indeed follows the picture outlined above, and discuss both the case where vortices encircle one another and the case where they interchange positions. In making this picture of non-Abelian statistics more precise, we define, starting from

each core state, further orthogonal single-particle states (“near-core states”) which are localized near a vortex core. The occupations of these additional single-particle states in the many-body ground states are also particle-hole symmetric and entangled between different vortices. In fact, we reveal a “self-similar” structure of the many-body wave function with respect to the occupation of these single-particle states which leads us to express the relation between our picture of non-Abelian statistics and the known representations of vortex braiding in the space of ground states^{10,13} in terms of compact operator identities.

The structure of this paper is as follows. We begin in Sec. II with a review of the description of the Pfaffian state as a p -wave superconductor, with vortices as quasiparticles. In Sec. III, we start with the definition of the single-particle states by introducing the “core states.” In Sec. IV, we explore the roles of quantum entanglement and geometric phases in the evolution of these superpositions when vortex positions are braided. The “near-core states” are introduced in Sec. V. The occupations of these “near-core states” in the many-body ground states is worked out in Sec. VI, revealing the “self-similar” structure of the wave functions. We conclude in Sec. VII. Some details are relegated to appendices.

II. SOLUTIONS OF BOGOLUBOV–DE GENNES EQUATIONS—REVIEW

The Pfaffian trial wave function for the quantized Hall state at Landau level filling factor $\nu=5/2$ was first introduced by Moore and Read⁷ as the first-quantized wave function

$$\Psi_{\text{MR}}(z_1, z_2, \dots) = \text{Pf} \left(\frac{1}{z_i - z_j} \right) \prod_{i < j} (z_i - z_j)^2 \prod_j e^{-(1/4l^2)|z_j|^2}, \quad (2)$$

where l is the magnetic length and $z_i = x_i + iy_i$ is the complex coordinate of the i th particle. For p particles (p an even integer), the Pfaffian in Eq. (2) takes the explicit form

$$\text{Pf} \left(\frac{1}{z_i - z_j} \right) = \frac{1}{2^{p/2}(p/2)!} \mathcal{A} \left\{ \frac{1}{z_1 - z_2} \frac{1}{z_3 - z_4} \dots \frac{1}{z_{p-1} - z_p} \right\}, \quad (3)$$

where \mathcal{A} is the antisymmetrization operator. It is instructive to view the Pfaffian appearing in the wave function in Eq. (2) as the real-space BCS wave function of composite fermions for a fixed number of particles.^{12,15} According to the associated pair wave function $g(z) = 1/z$, the pairing is of spinless (or spin-polarized) composite fermions in the $l=-1$ angular-momentum (p -wave) channel. The Pfaffian corresponds to a weakly paired superconductor, which for a two-dimensional p -wave superconductor is topologically distinct from the strongly paired phase.¹² The charged excitations of the quantum-Hall system are, in this description, the half-flux-quantum ($h/2e$) vortices of the superconductor.

As is often the case, the use of a first-quantization formulation is mathematically involved, and makes the physical picture difficult to read. The identification of the Pfaffian as a

complex p -wave BCS state of composite fermions subsequently led Read and Green¹² to introduce a second-quantization formulation which paved the way for a clearer physical picture. Their starting point is the BCS mean-field Hamiltonian

$$H = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) h_0 \psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \{ D * (\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) + D(\mathbf{r}, \mathbf{r}') \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \}, \quad (4)$$

with the single-particle term h_0 and the complex p -wave pairing function

$$D(\mathbf{r}, \mathbf{r}') = \Delta \left(\frac{\mathbf{r} + \mathbf{r}'}{2} \right) (i\partial_{x'} - \partial_{y'}) \delta(\mathbf{r} - \mathbf{r}'). \quad (5)$$

Read and Green¹² retain only the potential part of h_0 by setting $h_0 = -\mu(\mathbf{r})$ and argue that this is sufficient for studying the topological properties of the Pfaffian state, such as the statistics of its quasiparticles. In the presence of $2N$ vortices pinned at positions \mathbf{R}_i , the gap function takes the form $\Delta(\mathbf{r}) = |\Delta(\mathbf{r})| \exp[i\chi(\mathbf{r})]$ with $\chi(\mathbf{r}) = \sum_{i=1}^{2N} \arg(\mathbf{r} - \mathbf{R}_i)$. In the vicinity of vortex k , the phase $\chi(\mathbf{r})$ can be approximated by $\chi(\mathbf{r}) = \arg(\mathbf{r} - \mathbf{R}_k) + \Omega_k$ with $\Omega_k = \sum_{i \neq k}^{2N} \arg(\mathbf{R}_k - \mathbf{R}_i)$.

The fermionic excitations of superconductors are described by the Bogolubov–de Gennes (BdG) equations

$$E \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} -\mu(\mathbf{r}) & \frac{i}{2} \{ \Delta(\mathbf{r}), \partial_x + i\partial_y \} \\ \frac{i}{2} \{ \Delta * (\mathbf{r}), \partial_x - i\partial_y \} & \mu(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}. \quad (6)$$

For two-dimensional complex p -wave superconductors, solutions of nonzero energy should be distinguished from those of zero energy. We denote the nonzero energy solutions by $[u_E(\mathbf{r}), v_E(\mathbf{r})]$, with $u_E(\mathbf{r}) = v_{-E}^*(\mathbf{r})$. In second quantization, positive-energy solutions are associated with annihilation operators of BCS quasiparticles $\Gamma_E = \int d\mathbf{r} [u_E(\mathbf{r}) \psi(\mathbf{r}) + v_E(\mathbf{r}) \psi^\dagger(\mathbf{r})]$, while negative-energy solutions are associated with creation operators of the same quasiparticles $\Gamma_{-E} = \Gamma_E^\dagger$. The zero-energy solutions $[u_i(\mathbf{r}), v_i(\mathbf{r})]$ are localized at the vortex cores. For well-separated vortices, there is one such solution per vortex. With a choice of phase the advantages of which become clear below, these zero-energy solutions take the form

$$u_i(\mathbf{r}) = v_i^*(\mathbf{r}) = \frac{1}{\sqrt{2}} w_i^{(0)}(\mathbf{r}) e^{(i/2)\Omega_i}. \quad (7)$$

Here, the index $i=1, \dots, 2N$ numbers the vortices and the functions $w_i^{(0)}(\mathbf{r})$ are normalized wave functions localized near the core of the i th vortex. When the vortices are well separated, the functions $w_i^{(0)}(\mathbf{r})$ are mutually orthogonal. In Sec. V below, we iteratively define additional single-particle states localized in the vicinity of the vortex cores. These states will be denoted by $w_j^{(k)}(\mathbf{r})$, with the subscript labeling the vortex and the superscript enumerating the states near each vortex.

The zero-energy eigenstates of the BdG equations correspond to the Bogolubov operators

$$\gamma_j = \frac{1}{\sqrt{2}}[c_j e^{(i/2)\Omega_j} + c_j^\dagger e^{-(i/2)\Omega_j}], \quad (8)$$

where we introduced the operators $c_j = \int d\mathbf{r} w_j^{(0)}(\mathbf{r}) \psi(\mathbf{r})$ which annihilate particles in the vortex-core states $w_j^{(0)}(\mathbf{r})$. Evidently, $\gamma_j^\dagger = \gamma_j$ so that the operators associated with the zero-energy solutions are Majorana fermions.

The existence of the zero-energy solutions leads to a degeneracy of the ground state. Enumeration of the ground states is customarily done by combining the Majorana operators γ_i in pairs and defining (ordinary) fermionic creation and annihilation operators

$$\alpha_{2j}^\dagger = \frac{1}{\sqrt{2}}(\gamma_{2j-1} + i\gamma_{2j}) \quad (9)$$

with $j = 1, \dots, N$. The ground states can now be written in the occupation-number basis corresponding to these fermionic operators. A ground state $|\mathbf{m}\rangle$ is then labeled by the occupation numbers $\mathbf{m} = (m_2, m_4, \dots, m_{2N})$ with

$$\alpha_{2j}^\dagger \alpha_{2j} |\mathbf{m}\rangle = m_{2j} |\mathbf{m}\rangle \quad (10)$$

and

$$|\mathbf{m}\rangle = (\alpha_{2N}^\dagger)^{m_{2N}} \dots (\alpha_4^\dagger)^{m_4} (\alpha_2^\dagger)^{m_2} |\mathbf{m} = 0\rangle \quad (11)$$

leading to a 2^N -fold degeneracy of the ground state.

The BCS Hamiltonian (4) is diagonal when written in terms of the quasiparticle operators Γ_E and γ_i (Bogolubov transformation). The ground state is determined by the conditions $\Gamma_E |g.s.\rangle = 0$ for all $E > 0$. For a uniform superconductor in the absence of vortices (i.e., for space-independent Δ and μ), these equations lead to the celebrated BCS wave function $|\text{BCS}\rangle = \prod_{\mathbf{k}}' (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger) |\text{vac}\rangle$, where the prime indicates that pairs of momenta $(\mathbf{k}, -\mathbf{k})$ should be counted only once and $|\text{vac}\rangle$ is the state with no particles. In this case, the choice of a plane-wave basis for the single-particle states is natural.

In the presence of vortices, Δ and μ are space dependent, and there is no obvious single-particle basis for the description of the ground states. A proper choice of such a basis turns out to be helpful in our discussion of non-Abelian statistics.

III. CORE STATES

A natural starting point for a single-particle basis are the $2N$ states $w_i^{(0)}(\mathbf{r})$. These single-particle states, which we approximate to be orthogonal due to the large distance between the vortices, are associated with a 2^{2N} -dimensional subspace of the many-particle states. The remaining (infinitely-many) single-particle basis states remain unspecified throughout this section and are partially defined in Sec. V. We will refer to the first $2N$ single-particle states as the ‘‘vortex-core states,’’ and to the remaining single-particle states as the ‘‘other states.’’

Many-particle states in Fock space can now be expanded in terms of occupation numbers of these single-particle

states. A corresponding basis state of the Fock space is then written as

$$| \underbrace{1 \dots \dots 0}_{\text{vortex core}} \underbrace{0 \dots 1}_{\text{other}} \rangle, \quad (12)$$

where 0 (1) denotes an empty (occupied) state. The first factor has $2N$ digits and designates the occupations of the vortex-core states. We enumerate these states by $|\tau\rangle$ with $\tau = 0, \dots, 2^{2N} - 1$. Specifically, $|\tau=0\rangle$ denotes a many-body state in which all single-particle vortex-core states are unoccupied, i.e., a state that satisfies $c_j |\tau=0\rangle = 0$ for all j . The second factor in Eq. (12) designates the occupations of the ‘‘other states.’’ Below we find that for every possible ground state $|g.s.\rangle$ the probability to find the core states in an occupation $|\tau\rangle$ is equal to $1/2^{2N}$, and is independent of τ . A state in which this occupation depends on τ is necessarily an excited state.

Although the operators α_{2j} and α_{2j}^\dagger act on the occupations of the core states only, the quantum numbers \mathbf{m} do not fully label the 2^{2N} -dimensional space of states $|\tau\rangle$. In particular, there is no direct relation between the occupation numbers \mathbf{m} and the occupation of the single-particle states $w_j^{(0)}(\mathbf{r})$. In order to explore the structure of the ground states in terms of the states $|\tau\rangle$, we now introduce another set of quantum numbers associated with a second set of $2N$ Majorana operators

$$X_j = \frac{i}{\sqrt{2}}(c_j e^{(i/2)\Omega_j} - c_j^\dagger e^{-(i/2)\Omega_j}) \quad (13)$$

whose associated BdG spinors $[i w_j^{(0)}(\mathbf{r}) e^{(i/2)\Omega_j}, -i [w_j^{(0)}(\mathbf{r})]^* e^{-(i/2)\Omega_j}]$ are orthogonal by construction to the zero-energy solutions of the BdG equations. These operators obviously also act only on the occupations of the vortex-core states. However, when expanded over the complete set of BdG quasiparticle operators, they involve only nonzero energy quasiparticles so that

$$X_j = \sum_{E>0} [C_E^j \Gamma_E + C_E^{j*} \Gamma_E^\dagger] \quad (14)$$

with coefficients $C_E^j = i\sqrt{2} \int d\mathbf{r} u_E^*(\mathbf{r}) w_j^{(0)}(\mathbf{r}) e^{i\Omega_j/2}$. Upon pairing the vortices, these Majorana operators can again be combined to obtain (ordinary) fermionic operators¹⁶

$$\beta_{2j}^\dagger = \frac{1}{\sqrt{2}}(iX_{2j-1} + X_{2j}). \quad (15)$$

We label the occupation numbers of these fermions by x_2, x_4, \dots, x_{2N} , and introduce $\mathbf{x} = (x_2, x_4, \dots, x_{2N})$.

We now form a basis of the 2^{2N} -dimensional Fock subspace of the vortex-core states by defining

$$|\mathbf{m}, \mathbf{x}\rangle = (\alpha_{2N}^\dagger)^{m_{2N}} \dots (\alpha_4^\dagger)^{m_4} (\alpha_2^\dagger)^{m_2} (\beta_2^\dagger)^{x_2} (\beta_4^\dagger)^{x_4} \dots (\beta_{2N}^\dagger)^{x_{2N}} \times |\mathbf{m} = 0, \mathbf{x} = 0\rangle, \quad (16)$$

where $|\mathbf{m}=0, \mathbf{x}=0\rangle$ is the state annihilated by all the operators α_{2j} and β_{2j} . We obviously have $\langle \mathbf{m}, \mathbf{x} | \mathbf{m}', \mathbf{x}' \rangle = \delta_{\mathbf{m}, \mathbf{m}'} \delta_{\mathbf{x}, \mathbf{x}'}$. In terms of the occupations of the vortex-core states, the states $|\mathbf{m}, \mathbf{x}\rangle$ take the explicit form¹⁷

$$\begin{aligned}
 |\mathbf{m}, \mathbf{x}\rangle = s_{\mathbf{m}, \mathbf{x}} \prod_{j=1}^N \left\{ \frac{1}{\sqrt{2}} [1 + i(-1)^{x_{2j}}] \right. \\
 \times e^{-(i/2)(\Omega_{2j-1} + \Omega_{2j})} c_{2j-1}^\dagger c_{2j}^\dagger \delta_{m_{2j}, x_{2j}} \\
 \left. + \frac{1}{\sqrt{2}} [e^{-(i/2)\Omega_{2j-1}} c_{2j-1}^\dagger + i(-1)^{x_{2j}} e^{-(i/2)\Omega_{2j}} c_{2j}^\dagger] \right. \\
 \left. \times \delta_{m_{2j}, x_{2j}, 1} \right\} |\tau=0\rangle, \quad (17)
 \end{aligned}$$

where the vacuum $|\tau=0\rangle$ of the subspace of vortex-core states was defined above. The sign factor $s_{\mathbf{m}, \mathbf{x}} = \prod_{l=2}^N \prod_{r=1}^{l-1} (-1)^{x_{2l}(m_{2r} + x_{2r})}$ arises due to the different operator orderings in Eq. (16) and in the product in Eq. (17). Equation (17) is readily derived by first identifying the occupations of the vortex core states in $|\mathbf{m}=0, \mathbf{x}=0\rangle$ from the condition that this state is annihilated by all α_{2j} 's and β_{2j} 's. Subsequently, the occupations of the vortex-core states in the remaining states $|\mathbf{m}, \mathbf{x}\rangle$ can be obtained by successively applying creation operators α_{2j}^\dagger and β_{2j}^\dagger according to Eq. (16) and using Eqs. (8), (9), (13), and (15) in order to express these creation operators in terms of vortex-core operators.

A ground state labeled by \mathbf{m} is then a superposition of the form

$$|\mathbf{m}\rangle = \sum_{\mathbf{x}} |\mathbf{m}, \mathbf{x}\rangle |A_{\mathbf{x}}\rangle. \quad (18)$$

It is important to note that the states $|A_{\mathbf{x}}\rangle$ are *independent* of the particular ground state $|\mathbf{m}\rangle$. Arbitrary ground states $|\text{g.s.}, \alpha\rangle$ can be written as linear superpositions of the states $|\mathbf{m}\rangle$. Here and below we use the notation $|A\rangle$ to denote states in the Fock subspace corresponding to the unspecified ‘‘other states’’ in the single-particle basis. There are 2^N components in the superposition (18), one for every value of \mathbf{x} . The states $|A_{\mathbf{x}}\rangle$ should be determined by the requirement that the ground states are annihilated by all positive-energy annihilation operators Γ_E . Although we do not know the complete set of operators Γ_E , we can now show that

$$\langle A_{\mathbf{x}} | A_{\mathbf{x}'} \rangle = \frac{1}{2^N} \delta_{\mathbf{x}, \mathbf{x}'}. \quad (19)$$

To see that, we first note that since the operators X_j are composed of finite-energy quasiparticle operators only, the matrix element for any odd number of X operators between any two ground states must vanish. Thus,

$$\langle \text{g.s.}, \alpha | X_{j_1} | \text{g.s.}, \beta \rangle = \langle \text{g.s.}, \alpha | X_{j_1} X_{j_2} X_{j_3} | \text{g.s.}, \beta \rangle = \cdots = 0 \quad (20)$$

for arbitrary indices $\alpha, \beta, j_1, \dots$. Second, the matrix elements of a product of two *different* operators X_j between states in the ground-state manifold are

$$\begin{aligned}
 \langle \text{g.s.}, \alpha | X_{j_1} X_{j_2} | \text{g.s.}, \beta \rangle &= \delta_{\alpha\beta} \sum_{E>0} C_E^{j_1} C_E^{j_2*} \\
 &= 2 \delta_{\alpha\beta} \int d\mathbf{r} d\mathbf{r}' w_{j_1}^{(0)}(\mathbf{r}) [w_{j_2}^{(0)}(\mathbf{r}')]^* \\
 &\quad \times e^{(i/2)(\Omega_{j_1} - \Omega_{j_2})} \sum_{E>0} u_E^*(\mathbf{r}) u_E(\mathbf{r}'). \quad (21)
 \end{aligned}$$

For sufficiently high energies the functions $u_E(\mathbf{r})$ are approximately plane waves so that $\sum_E u_E^*(\mathbf{r}) u_E(\mathbf{r}')$ is a short-ranged function, presumably decaying exponentially with $|\mathbf{r} - \mathbf{r}'|$, even for nonuniform superconductors. Then, for well-separated vortices j_1 and j_2 , the matrix elements in Eq. (21) approximately vanish. Put in different words, the operation of the operators X_i is spatially localized around vortex i , and thus two such operators operating near two distant vortices generate orthogonal excitations. Similarly, the matrix element of any other even number of different X operators, taken with respect to any two ground states, vanishes as well. In Sec. V, we will also give a direct algebraic proof of this result which relies on a relation of the X_i to operators annihilating the ground states.

The conditions in Eqs. (20) and (21) imply some general conclusions regarding the states $|A_{\mathbf{x}}\rangle$, which we first present for the case of two vortices. There are four states $|\tau\rangle$, labeled by $|00\rangle, |01\rangle, |10\rangle, |11\rangle$.¹⁸ The phases encoding the vortex positions are related by $\Omega_2 = \Omega_1 + \pi$. The two ground states then take the explicit form

$$|\mathbf{m}=0\rangle = (|00\rangle - e^{-i\Omega_1} |11\rangle) |A_0\rangle + e^{-i\Omega_1/2} (|10\rangle - |01\rangle) |A_1\rangle, \quad (22)$$

$$|\mathbf{m}=1\rangle = (|00\rangle + e^{-i\Omega_1} |11\rangle) |A_1\rangle + e^{-i\Omega_1/2} (|10\rangle + |01\rangle) |A_0\rangle. \quad (23)$$

The condition $\langle \text{g.s.}, \alpha | X_i | \text{g.s.}, \alpha \rangle = 0$ implies that $\langle A_0 | A_1 \rangle = 0$. In addition, $\langle \text{g.s.}, \alpha | X_1 X_2 | \text{g.s.}, \alpha \rangle = 0$ imposes $\langle A_0 | A_0 \rangle = \langle A_1 | A_1 \rangle = 1/2$. Thus, while we cannot find the complete wave functions of the ground states without a full solution of the BdG equations, our procedure leads to the conclusion that the two ground states are incoherent superpositions of the states $(|00\rangle \pm e^{-i\Omega_1} |11\rangle)$ with the states $e^{-i\Omega_1/2} (|10\rangle \pm |01\rangle)$, with equal weights to both components. There is an equal probability 1/4 for all four possible charge arrangements $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. The parity of the particle number differs between the two basis vectors of the ground-state manifold. However, this difference in parity does not originate from the occupations of the two vortex-core states. A local measurement of one of the two vortex-core states cannot distinguish between the two ground states.

Generalizing to $2N$ vortices, it is easy to see that the requirement that the expectation value of products of X operators vanishes leads to Eq. (19). Thus, all basis functions of the ground-state manifold are an incoherent superposition of 2^N terms, of equal weight. Each of these terms is, by itself, a coherent superposition of 2^{2N-1} possible occupations of the core states, which constitute all possible occupations of a given parity. This observation clarifies why there are 2^N ground states, rather than 2^{2N} . Within the Fock space of the

core states there are 2^N eigenvectors for each eigenvalue \mathbf{m} , but a ground state is generated by their incoherent superposition, mixing all of them with equal weights.

The wave functions in Eq. (18) give an explicit description of the occupations of the core states. The operator $\hat{N}(w_i^{(0)}) \equiv (1/2)(\gamma_i + iX_i)(\gamma_i - iX_i)$ counts the number of particles in the i th core state. It is easy to see that

$$\langle \mathbf{m}' | \hat{N}(w_i^{(0)}) | \mathbf{m} \rangle = \langle \mathbf{m}' | [\hat{N}(w_i^{(0)})]^2 | \mathbf{m} \rangle = \frac{1}{2} \delta_{\mathbf{m}, \mathbf{m}'}. \quad (24)$$

Thus, in all possible ground states (including arbitrary superpositions of the states $|\mathbf{m}\rangle$) the occupation of each core state is particle-hole symmetric, with a probability of one half for being empty or occupied.

IV. GEOMETRIC PHASES AND QUANTUM ENTANGLEMENT IN THE EVOLUTION OF CORE STATES UNDER VORTEX BRAIDING

When vortices are adiabatically moved along closed trajectories, ending with braiding of their positions, the ground state may evolve in time away from the initial state, and the final ground state may thus be different from the initial one. There are, in principle, two contributions to this transformation of the ground state.¹⁹ The first originates from its explicit multiply valued dependence on the phases Ω_i (explicit monodromy). The second is through a non-Abelian geometric vector potential that gives rise to a non-Abelian Berry phase. As is always the case with geometric phases, only the sum of the explicit monodromy and the Berry phase is observable and one can split this sum between both contributions in any way desired by choice of appropriate phase factors. We now show that the phase choice we made in Eq. (7) makes the second contribution vanish, and proceed to calculate the first contribution.

We need to prove that the geometric vector potential²⁰

$$\text{Im} \langle \mathbf{m} | \nabla_{\mathbf{R}_i} | \mathbf{m}' \rangle \quad (25)$$

vanishes for all $\mathbf{m}, \mathbf{m}', \mathbf{R}_i$. The states $|\mathbf{m}\rangle$ depend on \mathbf{R}_i through the phases Ω_i and through the functions $w_i^{(0)}(\mathbf{r})$. Since the $w_i^{(0)}(\mathbf{r})$ are real (up to some trivial global phase factor), their derivative does not contribute in Eq. (25), and we may write $\nabla_{\mathbf{R}_i} = \sum_j (\nabla_{\mathbf{R}_j} \Omega_j) (\partial / \partial \Omega_j)$ and compute the matrix element

$$\begin{aligned} \langle \mathbf{m} | \frac{\partial}{\partial \Omega_j} | \mathbf{m}' \rangle &= \delta_{\mathbf{m}\mathbf{m}'} \sum_{\mathbf{x}} \langle A_{\mathbf{x}} | \frac{\partial}{\partial \Omega_j} | A_{\mathbf{x}} \rangle \\ &+ \frac{1}{2^N} \sum_{\mathbf{x}} \langle \mathbf{m}, \mathbf{x} | \frac{\partial}{\partial \Omega_j} | \mathbf{m}', \mathbf{x} \rangle. \end{aligned} \quad (26)$$

The first term on the right-hand side is diagonal in \mathbf{m}, \mathbf{m}' and otherwise independent of \mathbf{m} . It therefore leads only to Abelian phase factors. Using the explicit states in Eq. (17) one finds that also the diagonal elements $\mathbf{m} = \mathbf{m}'$ of the second term are independent of \mathbf{m} . The only contribution to the non-Abelian part of the Berry phase can therefore arise due to the off-diagonal contributions $\mathbf{m} \neq \mathbf{m}'$ of the second term. How-

ever, these vanish as one may verify by using the explicit states in Eq. (17). Thus, when the wave functions are written as in Eqs. (17) and (18) the only phase factors that lead to non-trivial unitary transformations arise from the explicit dependence of these wave functions on the phases Ω_i .

More explicitly, Eq. (17) shows that the part of the wave function in which the core state i is occupied has an amplitude proportional to $e^{-i\Omega_i/2}$, while the part in which this state is empty does not depend on Ω_i . Since the ground states involve superpositions of empty and occupied core states, when the phase Ω_i accumulates a 2π shift, a relative minus sign is introduced between the components of the superpositions in which core state i is empty and occupied, and the ground state does not necessarily come back to itself. The source of the evolution from one ground state to another is then in the phases between different components of the wave function, and not in any change of occupation of states.

It is instructive to examine in detail the case of the i th vortex encircling the j th vortex, for which

$$\Omega_i \rightarrow \Omega_i + 2\pi, \quad \Omega_j \rightarrow \Omega_j + 2\pi. \quad (27)$$

This change of phase affects both the states $|\mathbf{m}, \mathbf{x}\rangle$ and the states $|A_{\mathbf{x}}\rangle$, according to

$$|\mathbf{m}, \mathbf{x}\rangle \rightarrow (2i\gamma_i X_i)(2i\gamma_j X_j) |\mathbf{m}, \mathbf{x}\rangle, \quad (28)$$

$$|A_{\mathbf{x}}\rangle \rightarrow \hat{B}_{ij} |A_{\mathbf{x}}\rangle, \quad (29)$$

where \hat{B}_{ij} is an operator that acts on the “other”, non-core, states, only. The final state $\sum_{\mathbf{x}} (2i\gamma_i X_i)(2i\gamma_j X_j) |\mathbf{m}, \mathbf{x}\rangle \hat{B}_{ij} |A_{\mathbf{x}}\rangle$ must be a ground state. However, the operators X_i, X_j generate excitations above the ground states. The operator \hat{B}_{ij} must then be an operator that annihilates these excitations. More precisely, since the states $|A_{\mathbf{x}}\rangle$ do not depend on \mathbf{m} , the operator $X_i X_j \hat{B}_{ij}$ must be a c number within the subspace of ground states. In fact, for the norm of the ground state to be conserved during the braiding of vortices, the magnitude of this c number must be unity, i.e.,

$$2X_i X_j \hat{B}_{ij} = e^{i\phi_a} \quad (30)$$

with ϕ_a being an Abelian phase. In this way, we recover the known unitary transformation for winding of two vortices $2\gamma_i \gamma_j$ given in Eq. (1) [see also Appendix A]. This shows that despite the appearance of Eq. (1), this transformation does not involve any changes of core-state occupations, but only changes in relative phases between the components of a superposition, each of which has different core-state occupations.

In the subsequent sections, we will study the states $|A_{\mathbf{x}}\rangle$ much more explicitly by introducing the “near-core” single-particle states. We will find that these states are structurally very similar to the ground states $|\mathbf{m}\rangle$ and this allows us to give explicit expressions for the operators \hat{B}_{ij} (up to an Abelian phase factor). These expressions do indeed satisfy Eq. (30).

The above observations allow us to conclude that the ground states spanned by the basis in Eq. (18) are states in which the occupation of the core states at different vortices

are fully entangled, in the following sense: There is no ground state of the system in which the parity of the number of particles is well defined, and in which the occupations of two subsets of core states are disentangled from one another. If such a state were to exist, its wave function could be written as

$$\hat{C}_1 \hat{C}_2 \hat{C}_3 |\text{vac}\rangle, \quad (31)$$

where \hat{C}_1 is an operator that acts only on the core states belonging to the first subset, \hat{C}_2 is an operator that acts only on core states belonging to the second subset, and \hat{C}_3 is an operator that acts solely on the remaining states (core states or other states) not included in any of the two subsets. However, for the state in Eq. (31) to have well-defined particle-number parity, the states created by \hat{C}_1 or \hat{C}_2 must each have definite parity. By considering the effect of an encircling in which one vortex (say, the i th vortex) from the first subset winds around another vortex of the second subset (say, the j th vortex), we find that this cannot happen. The unitary transformation $2\gamma_i\gamma_j$ corresponding to this transformation changes the parity of the particle number for both the first and the second subset, while we showed that the transformation of the ground state is a consequence of changes in phases only, rather than changes in core states occupation. Consequently, a state of the form in Eq. (31) cannot be a ground state.

In some sense, the entanglement of the occupations of core states is signaled by Eq. (10). As seen from that equation, the ground states $|\gamma_{2j-1}\mathbf{m}\rangle$ and $|\gamma_{2j}\mathbf{m}\rangle$ differ from one another only by a phase factor, despite the fact that they are obtained from the ground state $|\mathbf{m}\rangle$ by the application of two Majorana operators localized very far from one another.

Interestingly, despite the entanglement, the occupations of different core states i and j are uncorrelated,

$$\begin{aligned} &\langle \text{g.s.} | \hat{N}(w_i^{(0)}) \hat{N}(w_j^{(0)}) | \text{g.s.} \rangle \\ &= \langle \text{g.s.} | \hat{N}(w_i^{(0)}) | \text{g.s.} \rangle \langle \text{g.s.} | \hat{N}(w_j^{(0)}) | \text{g.s.} \rangle = \frac{1}{4}. \end{aligned} \quad (32)$$

This lack of correlations persists also to higher-order correlators.

Furthermore, we can conclude that the total number of particles in the core states, counted by the operator $\hat{N}_{\text{core}} = \sum_{i=1}^{2N} \hat{N}(w_i^{(0)})$, does not have a well-defined parity. Rather, it has equal probabilities for being even and odd, irrespective of what is the parity of the total number of particles in the ground state. To see that, we consider the particle-number parity operator $\exp(i\pi\hat{N}_{\text{core}})$. Due to the lack of correlations between different vortices

$$\langle \text{g.s.} | \exp(i\pi\hat{N}_{\text{core}}) | \text{g.s.} \rangle = \prod_{j=1}^{2N} \langle \text{g.s.} | \exp[i\pi\hat{N}(w_j^{(0)})] | \text{g.s.} \rangle = 0. \quad (33)$$

Thus, the parity of the ground states cannot be determined by a measurement of the occupation of the core states alone.

Despite the inherent quantum entanglement of the ground states, it appears impossible to formulate corresponding Bell inequalities. Each core state defines a two-dimensional Hilbert space, similar to a spin- $\frac{1}{2}$. However, the operators associated with these spaces at different cores, the *fermionic* operators γ_j and X_j , do not commute. Thus, their classical analogs are ill defined.²¹

What happens when two vortices are interchanged can be analyzed along similar lines to the case of one vortex encircling another. We now analyze the case of interchanging vortices from the same pair, $2i-1$ and $2i$. Note that choosing the vortices from the same pair does not imply any loss of generality, both because for any interchange we can choose a pairing such that the two vortices are from the same pair, and because our considerations will eventually lead to an operator expression which is independent of the particular choice of pairing.

As the adiabatic motion of vortices does not involve any tunneling of particles between vortex cores, an interchange of the position of vortices interchanges the occupation of their core states. When both core states are occupied, the interchange is accompanied by a factor of (-1) , since two fermions interchange positions. In addition, one of the vortices necessarily crosses the cut line of the phase of the other, changing this phase by 2π (see Appendix A). The phase of the other vortex remains intact. Implementing these transformations in Eq. (17), the term $[1 + i(-1)^{x_{2j}} e^{-i(\Omega_{2j-1} + \Omega_{2j})/2} c_{2j-1}^\dagger c_{2j}^\dagger]$ remains unaffected by the interchange, while the relative sign between the two components changes in the term $[e^{-i\Omega_{2j-1}/2} c_{2j-1}^\dagger + i(-1)^{x_{2j}} e^{-i\Omega_{2j}/2} c_{2j}^\dagger]$.

These transformations of the core-state wave functions are implemented by the operator $e^{\pi\gamma_{2j-1}\gamma_{2j}/2} e^{\pi X_{2j-1}X_{2j}/2}$, acting on Eq. (17). By contrast, as found in Ref. 13 (reviewed in Appendix A), the unitary transformation that enacts the vortex interchange on the states in Eq. (18) is $e^{\pi\gamma_{2j-1}\gamma_{2j}/2}$. As in the case of encircling, the difference between these two transformations is an operator \hat{B} that acts on the $|A_x\rangle$ part of the wave function in Eq. (18).

The states $|A_x\rangle$ together with the operators \hat{B} that act on them when vortices wind and interchange are the subject of the following sections. We define a set of single-particle states adjacent to the core state for each vortex (“near-core states”), and show that the operator \hat{B} affects the occupation of these states in exactly the same way as the operators $2\gamma_i\gamma_j$ and $e^{\pi\gamma_{2j-1}\gamma_{2j}/2}$ affect the occupation of the core states for vortex winding and encircling, respectively. In fact, we find the corresponding operators \hat{B} to have the same functional forms, but with the Majorana operators γ_i and γ_j replaced by analogous Majorana operators associated with the near-core states. We explain this in terms of a “self-similar” structure of the ground-state wave functions.

V. STATES NEAR THE CORE

Our information on the states $|A_x\rangle$ introduced in Eq. (18) has so far relied on the conditions in Eqs. (20) and (21) for matrix elements of products of the operators X_i . These operators were constructed to have two main virtues. (i) They

create and annihilate particles in the core states only. (ii) They create and annihilate only excitations (Bogolubov quasiparticles) with $E > 0$. We now take these operators as a starting point in a scheme by which we define the set of mutually orthogonal single-particle states $w_i^{(k)}(\mathbf{r})$, where the subscript i refers to the vortex number and the superscript k enumerates the iterations in our scheme. The new single-particle states remain localized near the vortex cores and provide insight into the nature of the states $|A_{\mathbf{x}}\rangle$.

We get to these states by using the X_i 's to construct a set of operators $Y_i^{(k)}$ that, unlike the Majorana X_i 's, annihilate the ground states

$$Y_i^{(k)}|\mathbf{m}\rangle = 0 \quad (34)$$

for all i, k, \mathbf{m} . Furthermore, these operators anticommute $\{Y_i^{(k)}, Y_{i'}^{(k')}\} = 0$ and each operator $Y_i^{(k)}$ creates and annihilates particles only in the two basis states $w_i^{(k-1)}(\mathbf{r})$ and $w_i^{(k)}(\mathbf{r})$. By virtue of the conditions in Eq. (34), these operators specify the ground-state wave functions in the subspace spanned by the states $w_i^{(k)}(\mathbf{r})$.

Our scheme starts from the expansion of the operators X_i in Eq. (14). We define the two sets of operators

$$Y_i^{(1)} = \sqrt{2} \sum_{E>0} C_E^i \Gamma_E, \quad (35)$$

$$Z_i^{(1)} = i \sum_{E>0} (C_E^i \Gamma_E - C_E^{i*} \Gamma_E^\dagger). \quad (36)$$

The operators $Y_i^{(1)}$ annihilate all the ground states since they are constructed from (positive-energy) annihilation operators only. The operators $Z_i^{(1)}$ are, by construction, Majorana operators, and can thus be written as

$$Z_i^{(1)} = \frac{1}{\sqrt{2}} \int d\mathbf{r} [w_i^{(1)}(\mathbf{r}) \psi(\mathbf{r}) + \text{H.c.}]. \quad (37)$$

This defines a set of $2N$ single-particle states $w_i^{(1)}(\mathbf{r})$. We prove in Appendix B that for well separated vortices the $w_i^{(1)}(\mathbf{r})$ are mutually orthogonal as well as orthogonal to the core states $w_i^{(0)}(\mathbf{r})$. Thus, we can extend our single-particle basis by adding to it the $2N$ states $w_i^{(1)}(\mathbf{r})$. Note that for conciseness of notation, we absorb the phase factors $\exp(i\Omega_i/2)$ into the definition of the states $w_i^{(k)}(\mathbf{r})$ throughout this section. We comment below on how they should be reinstated.

Since $X_i = (1/\sqrt{2})[Y_i^{(1)} + Y_i^{(1)\dagger}]$, the condition

$$Y_i^{(1)}|g.s., \alpha\rangle = 0 \quad (38)$$

implies immediately that any combination of different operators X_i has zero matrix elements between ground states as required in Sec. III. Using the relation $Y_i^{(1)} = (1/\sqrt{2})(X_i - iZ_i^{(1)})$, we can write

$$Y_i^{(1)} = \frac{i}{2} \int d\mathbf{r} \{ [w_i^{(0)}(\mathbf{r}) - w_i^{(1)}(\mathbf{r})] \psi(\mathbf{r}) - ([w_i^{(0)}(\mathbf{r})]^* + [w_i^{(1)}(\mathbf{r})]^*) \psi^\dagger(\mathbf{r}) \}. \quad (39)$$

Thus, these $2N$ operators affect the occupations of the states $w_i^{(0)}(\mathbf{r})$ and $w_i^{(1)}(\mathbf{r})$ only.

To iterate this process it is helpful to summarize the steps leading to the definition of $w_i^{(1)}(\mathbf{r})$ through $Y_i^{(1)}$, using the concise spinor representation for the operators. We start with the operators $\gamma_i = (1/\sqrt{2})(w_i^{(0)}(\mathbf{r}), [w_i^{(0)}(\mathbf{r})]^*)$ in Eq. (8) which act on the occupation of the $w_i^{(0)}(\mathbf{r})$ only. In Eq. (13) we define the operators $X_i = i\sigma_z \gamma_i = (1/\sqrt{2})(iw_i^{(0)}(\mathbf{r}), -i[w_i^{(0)}(\mathbf{r})]^*)$ acting on the occupations of the same single-particle states (σ_z is a Pauli matrix). By construction, the spinors corresponding to X_i are orthogonal to those corresponding to γ_i , implying that the corresponding operators anticommute. Then, in Eq. (35), we extract from the operators X_i the parts $Y_i^{(1)}$ that annihilate the ground state. The operators Y_i , in turn, are written in Eqs. (36)–(39) as sums of Hermitian operators X_i and anti-Hermitian operators $iZ_i^{(1)}$, and finally, we defined $w_i^{(1)}(\mathbf{r})$ through the Majorana operators $Z_i^{(1)}$. In spinor representation, these last three steps can be recast as $Z_i^{(1)} = -S\sigma_z\gamma_i$ with

$$S = \sum_{E \neq 0} \text{sgn } E \begin{vmatrix} u_E \\ v_E \end{vmatrix} \begin{vmatrix} u_E \\ v_E \end{vmatrix}^\dagger. \quad (40)$$

The operator S is a difference of two projection operators. The positive (negative) energy part of the sum projects to the subspace of positive (negative) energy BdG solutions.

We now iterate this process to define states $w_i^{(k)}(\mathbf{r})$ and a set of operators $Y_i^{(k)}$ for which $Y_i^{(k)}|g.s., \alpha\rangle = 0$. This is achieved by generating the set of Majorana operators

$$Z_i^{(k)} = \frac{1}{\sqrt{2}} \begin{pmatrix} w_i^{(k)}(\mathbf{r}) \\ [w_i^{(k)}(\mathbf{r})]^* \end{pmatrix} = [-S\sigma_z]^k \gamma_i. \quad (41)$$

When writing out S explicitly in real space representation, according to Eq. (40), it contains energy sums of the type that has been discussed following Eq. (21). By the same arguments employed there, we can conclude that as a function of the two coordinates \mathbf{r} and \mathbf{r}' , the operator S is short ranged, i.e., decays fast for large $|\mathbf{r} - \mathbf{r}'|$. Thus, $w_i^{(k)}(\mathbf{r})$ is also localized around the i th vortex although its extent from the vortex core increases with k . Since the construction assumes that states $w_i^{(k)}(\mathbf{r})$ localized around different vortices do not overlap, there exists an upper limit to the number of iterations. We denote the last iteration number by L .

The functions $w_i^{(k)}(\mathbf{r})$ are studied in more detail in Appendix B. We find that for iterations $k < L$, the various $w_i^{(k)}(\mathbf{r})$ are mutually orthogonal,

$$\langle w_i^{(k)} | w_j^{(k')} \rangle = \delta_{ij} \delta_{kk'}. \quad (42)$$

As long as the spatial extent of the states $w_i^{(k)}(\mathbf{r})$ is small compared to the distance between vortices, the dependence of the near-core states $w_i^{(k)}(\mathbf{r})$ on the phases Ω_i is analogous

to that of the core states. Specifically, these phases can be made explicit by the replacement

$$w_i^{(k)}(\mathbf{r}) \rightarrow w_i^{(k)}(\mathbf{r})e^{i\Omega_i/2}. \quad (43)$$

This can be seen from Eqs. (40) and (41) in combination with the observation that for \mathbf{r} in the vicinity of vortex i , all finite-energy BdG solutions $u_E(\mathbf{r})$ and $v_E(\mathbf{r})$ depend on the vortex positions through the phase factor $e^{i\Omega_i/2}$.

We also define

$$X_i^{(k)} = \frac{1}{\sqrt{2}} \begin{pmatrix} iw_i^{(k)}(\mathbf{r}) \\ -i[w_i^{(k)}(\mathbf{r})]^* \end{pmatrix} \quad (44)$$

and the operators

$$\begin{aligned} Y_i^{(k)} &= \frac{1}{\sqrt{2}}[X_i^{(k-1)} - iZ_i^{(k)}] \\ &= \frac{i}{\sqrt{2}}(1+S)\sigma_z Z_i^{(k-1)} \\ &= \frac{i}{2}[(c_i^{(k-1)} - c_i^{(k)}) - (c_i^{(k-1)\dagger} + c_i^{(k)\dagger})] \end{aligned} \quad (45)$$

which annihilate the ground states [see Eq. (34)]. Here, the operators $c_i^{(k)}$ annihilate particles in the states $w_i^{(k)}(\mathbf{r})$. This iterative construction enlarges our single-particle basis. Starting with the $2N$ core states $w_i^{(0)}(\mathbf{r})$, we defined an additional $L-1$ ‘‘near-core’’ states for every vortex.

The occupations of the newly defined $L-1$ ‘‘near-core’’ states are all particle-hole symmetric. This can be seen by noting that the operator $\hat{N}(w_i^{(k)}) = (1/2)(Z_i^{(k)} + iX_i^{(k)})(Z_i^{(k)} - iX_i^{(k)})$ counts the number of particles in the state $w_i^{(k)}(\mathbf{r})$. Since

$$\hat{N}(w_i^{(k)}) = \frac{1}{2} + iX_i^{(k)}Z_i^{(k)} = \frac{1}{2}[1 + (Y_i^{(k+1)\dagger} + Y_i^{(k+1)})(Y_i^{(k)\dagger} - Y_i^{(k)})] \quad (46)$$

and since the operators $Y_i^{(k)\dagger}$ and $Y_i^{(k+1)}$ correspond to orthogonal excitations, one finds

$$\langle \mathbf{m}' | \hat{N}(w_i^{(k)}) | \mathbf{m} \rangle = \langle \mathbf{m}' | [\hat{N}(w_i^{(k)})]^2 | \mathbf{m} \rangle = \frac{1}{2} \delta_{\mathbf{m}, \mathbf{m}'}. \quad (47)$$

In the next section we solve Eq. (34) to extract the ground-state wave functions in the Fock subspace spanned by the near-core states $w_i^{(k)}(\mathbf{r})$.

VI. GROUND-STATE WAVE FUNCTIONS AND NON-ABELIAN STATISTICS

Solving Eq. (34), we now show that the structure we found in Sec. III for the occupations of the core states repeats itself for the near-core states. This allows us to complete the argument that the effect of vortex braiding can be understood explicitly in terms of the geometric phases Ω_i .

The detailed form of the ground-state wave function depends on the convention for the order in which creation operators of various states act on the vacuum. Equation (18)

positions all creation operators for the core states to the left of creation operators for other states, and Eq. (16) specifies the order in which core states are being filled. In that spirit, the creation operators for the first iteration of near-core states $w_i^{(1)}(\mathbf{r})$ are going to be positioned to the right of those of the core states, and so on with increasing number of the iteration. Within each iteration, we follow the convention defined in Eq. (16) for the core states.

We first determine the occupations of the near-core states of the first iteration, $w_i^{(1)}(\mathbf{r})$ in the states $|A_{\mathbf{x}}\rangle$. To this end, we define creation and annihilation operators from pairs of the operators $Z_i^{(1)}$ and $X_i^{(1)}$,

$$\delta_{2j} = \frac{1}{\sqrt{2}}(Z_{2j-1}^{(1)} - iZ_{2j}^{(1)}), \quad (48)$$

$$\eta_{2j} = \frac{1}{\sqrt{2}}(-iX_{2j-1}^{(1)} + X_{2j}^{(1)}). \quad (49)$$

Then we can express the states $|A_{\mathbf{x}}\rangle$ in terms of the states

$$\begin{aligned} |\mathbf{m}, \mathbf{x}\rangle^{(1)} &= (\delta_{2N}^\dagger)^{m_{2N}} \cdots (\delta_4^\dagger)^{m_4} (\delta_2^\dagger)^{m_2} (\eta_{2j}^\dagger)^{x_2} (\eta_4^\dagger)^{x_4} \cdots (\eta_{2N}^\dagger)^{x_{2N}} \\ &\times |\mathbf{m} = 0, \mathbf{x} = 0\rangle^{(1)}, \end{aligned} \quad (50)$$

where the superscript on the state indexes the iteration. The conditions $(Y_{2j-1}^{(1)} \pm iY_{2j}^{(1)})|\mathbf{m}\rangle = 0$ for the ground states can be rewritten as [see Eq. (45)]

$$(\beta_{2j} - \delta_{2j}^\dagger)|\mathbf{m}\rangle = 0, \quad (51)$$

$$(\beta_{2j}^\dagger + \delta_{2j})|\mathbf{m}\rangle = 0. \quad (52)$$

Applying these conditions to the ground states, we find

$$|A_{\mathbf{x}}\rangle = \sum_{\mathbf{x}'} |\mathbf{x}, \mathbf{x}'\rangle^{(1)} |A_{\mathbf{x}'}\rangle^{(1)}, \quad (53)$$

in terms of further states $|A_{\mathbf{x}'}\rangle^{(1)}$ which contain the occupations of the remaining near-core states as well as the other states. As expected, Eq. (53) satisfies Eq. (19). Iterating this procedure, we get

$$|A_{\mathbf{x}}\rangle^{(1)} = \sum_{\mathbf{x}'} |\mathbf{x}, \mathbf{x}'\rangle^{(2)} |A_{\mathbf{x}'}\rangle^{(2)}, \quad (54)$$

and so on, as long as near-core states from different vortices do not overlap. Consequently, we can write the ground-state wave functions as

$$\begin{aligned} |\mathbf{m}\rangle &= \sum_{\mathbf{x}^{(0)}} |\mathbf{m}, \mathbf{x}^{(0)}\rangle^{(0)} \sum_{\mathbf{x}^{(1)}} |\mathbf{x}^{(0)}, \mathbf{x}^{(1)}\rangle^{(1)} \\ &\times \sum_{\mathbf{x}^{(2)}} |\mathbf{x}^{(1)}, \mathbf{x}^{(2)}\rangle^{(2)} \cdots \sum_{\mathbf{x}^{(L)}} |\mathbf{x}^{(L-1)}, \mathbf{x}^{(L)}\rangle^{(L)} |A_{\mathbf{x}^{(L)}}\rangle^{(L)}. \end{aligned} \quad (55)$$

This structure of the ground states is helpful for analyzing the effect of vortex braiding.

As discussed in Sec. IV, the effect of encircling vortex i by vortex j on the ground states $|\mathbf{m}\rangle$ is given by the unitary transformation $2\gamma_i\gamma_j$ [Eq. (1)]. In Eqs. (28) and (29), we decomposed this transformation into two factors, one affect-

ing the core states, and the other affecting the other states.

The “self-similarity” of the wave function, evident in Eqs. (53)–(55), suggests that the effect of vortex encircling on the states $|A_{\mathbf{x}}\rangle$ is analogous to its effect on the ground states $|\mathbf{m}\rangle$ themselves. Clearly, the analog of the operators γ_i in the first generation of near-core states are the operators $Z_i^{(1)}$. Thus, one expects

$$\hat{\mathcal{B}}_{ij} = 2Z_i^{(1)}Z_j^{(1)} \quad (56)$$

and the associated operator identity

$$2\gamma_i\gamma_j = (2i\gamma_iX_i)(2i\gamma_jX_j)(2Z_i^{(1)}Z_j^{(1)}) \quad (57)$$

when applied to any ground state. Indeed, the proof of this identity follows from the fact that $Y_i = (1/\sqrt{2})(X_i - iZ_i^{(1)})$ annihilates any ground states so that, when acting within the subspace of ground states, one has $0 = \sqrt{2}X_iY_i = 1/2 - iX_iZ_i^{(1)}$ or $2iX_iZ_i^{(1)} = 1$.

An analogous picture emerges for the exchange of vortices. Here, we found that the explicit effect of exchange on the states $|\mathbf{m}, \mathbf{x}\rangle$ is equivalent to the action of the operator $\exp\{\pi\gamma_i\gamma_j/2\}\exp\{\pi X_iX_j/2\}$. On the other hand, the effect of the interchange on the ground states is given by the operator $\exp\{\pi\gamma_i\gamma_j/2\}$. Due to the “self-similarity” of the wave function, the connection between these two operators is expected to be furnished by

$$\hat{\mathcal{B}} = \exp\{\pi Z_i^{(1)}Z_j^{(1)}/2\}. \quad (58)$$

Indeed, there exists a corresponding operator identity

$$\exp\{\pi\gamma_i\gamma_j/2\} = \exp\{\pi\gamma_i\gamma_j/2\}\exp\{\pi X_iX_j/2\}\exp\{\pi Z_i^{(1)}Z_j^{(1)}/2\} \quad (59)$$

valid when acting within the subspace of ground states. Its proof uses the same ingredients as in the case of encircling.

For both vortex encircling and exchange, this procedure can now be repeated for the near-core states obtained in higher iterations. In this way, it follows that the effect of vortex encircling or exchange on any core or near-core states is entirely contained in the geometric phases Ω_i .

This discussion clarifies the difference between unitary transformations composed of zero-energy Majorana operators, say, $\gamma_{2j-1}\gamma_{2j}$, and unitary transformations composed of nonzero energy Majorana operators, such as $X_{2j-1}^{(k)}X_{2j}^{(k)}$ and $Z_{2j-1}^{(k)}Z_{2j}^{(k)}$. When acting on a ground state, the first one leaves the system within the subspace of ground states, while the last two excite the system. Any unitary transformation that may be implemented by means of an adiabatic vortex braiding leaves the system in the ground state subspace. That is the case for $\gamma_{2j-1}\gamma_{2j}$, whose effect on a ground state may be reduced to a series of phase changes associated with vortex braiding. By contrast, the effect of the other two operators may not be implemented by an adiabatic braiding of vortices.

The number of generations L appearing in Eq. (55) is chosen such that the states $w_i^{(k)}(\mathbf{r})$ generated by our iterative process do not become extended enough to overlap. If the iterative process is carried out further, states from different vortices start overlapping, and therefore cannot be used as basis states in a single-particle basis. In principle, these states

may be orthogonalized by means of a Gram-Schmidt-type process. The states resulting from that process, however, would not necessarily share the properties of the states $w_i^{(k)}(\mathbf{r})$ for $k < L$, namely, their occupation may not be particle-hole symmetric, and the way they are affected by vortex braiding may be different.

VII. SUMMARY

The composite-boson theory of the fractional quantum Hall effect at filling fractions $\nu = 1/m$ (m odd) employs a Chern-Simons transformation to map the electronic system to a superfluid of composite bosons. It explains the fractional statistics of the excitations of these states by describing them as charged vortices in that superfluid, and the statistical phase as the effect of the charge of one vortex on the geometric phase accumulated by another vortex as it moves adiabatically.

The Moore-Read theory describes the $\nu = 5/2$ state also as a superfluid. Again, charged excitations are vortices in this superfluid, and these vortices accumulate geometric phases as they move. However, in this case the effective bosons forming the superfluid are Cooper pairs of composite fermions. As a consequence, this state has excitation modes that involve the breaking of Cooper pairs into two composite fermions. These modes are solutions of the Bogolubov–de Gennes equations. In the presence of well-separated vortices, each vortex gives rise to one zero-energy solution. These zero-energy solutions represent Majorana operators, operating on the core state of their vortex. For $2N$ vortices, these zero modes lead to a 2^N -fold degeneracy of the ground state in the presence of vortices. The $2N$ core states define a 2^{2N} -dimensional Fock space, since each core state may be occupied or empty. We found that each ground state has an equal probability for each of the 2^{2N} possibilities to occupy the core states, and that the way these possibilities are superposed is such that (at least for ground states with a definite parity of the total particle number) the occupation of core states in one vortex is entangled with the occupations of all core states in all other vortices. We showed that it is the relative phases between the amplitudes for different occupations that distinguishes between the various ground states, and that it is these relative phases that vary as the vortices move. This allows the system to transform between ground states due to vortex braiding. It is interesting to observe that unlike the case of ordinary quantized Hall states, there seems to be no direct relation between the charge carried by the vortices and their non-Abelian statistics.

While the zero-energy Majorana modes affect only the occupations of the core states of the vortices, we showed that it is possible to extract some general information regarding the occupations of other single-particle states without explicitly solving the Bogolubov–de Gennes equations. In particular, we constructed a set of single-particle states which are localized near the vortex cores and whose occupations are also maximally uncertain (all possibilities of their occupations are equally probable) and maximally entangled. The definition of these near-core states allowed us to explicitly relate our picture of non-Abelian statistics, based on en-

tanglement and geometric phases, to previously existing approaches based on representations of vortex braiding in terms of unitary transformations that create and annihilate particles in the core states. The elucidation of the role of quantum entanglement and geometric phases may be useful for understanding the effect of decoherence on non-Abelian statistics, a question which is of relevance in the context of topological quantum computation.²²

The Moore-Read state is only the simplest example of proposed FQHE wave functions²³ whose excitations satisfy non-Abelian statistics. As in this example, non-Abelian statistics is generally associated with a degeneracy of the ground state. However, the other proposed states lack a description in terms of second quantization, and in the absence of such a description it is hard to generalize our analysis for the Moore-Read state to the entire set of non-Abelian states. We believe, however, that a second-quantization formulation of other non-Abelian states would lead to a similar picture.

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APPENDIX A: UNITARY TRANSFORMATIONS FOR VORTEX ENCIRCLING AND INTERCHANGE

In this appendix, we review for completeness how to construct the unitary transformations U associated with particle exchange and encircling.¹³ For this purpose, we analyze the time evolution of the many-particle state within the degenerate subspace of ground states as the vortices adiabatically traverse trajectories that start and end in the same set of positions. The unitary transformation is defined by the relation between the final state $|\psi(t=T)\rangle$ and the initial state $|\psi(t=0)\rangle$,

$$|\psi(t=T)\rangle = U|\psi(t=0)\rangle. \quad (\text{A1})$$

Correspondingly, the time evolution of the operators γ_i spanning the degenerate subspace is given by

$$\gamma_i(t=T) = U\gamma_i(t=0)U^\dagger. \quad (\text{A2})$$

The time evolution of the operators γ_i can be readily read off from their definition (8) and the explicit form (7) of the zero-energy spinors of the Bogolubov–de Gennes equations. This can be used to identify the operators U up to an Abelian phase. We note that with our choice of phase for the zero-energy spinors in Eq. (7), their Berry phase during adiabatic phase evolution vanishes and the phase evolution is given

solely by the explicit monodromy. Before constructing U for exchange trajectories or encircling, we first construct unitary operators from the set of γ_i 's which are helpful in giving an explicit expression for the operators U .

The unitary transformation $u_k = \sqrt{2}\gamma_k$ adds a minus sign to all operators γ_j with $j \neq k$. If $j=k$, it leaves the operator unchanged:

$$u_k \gamma_j u_k^\dagger = \begin{cases} \gamma_k & \text{when } j=k, \\ -\gamma_j & \text{otherwise.} \end{cases} \quad (\text{A3})$$

Obviously $\{u_k, u_{k'}\} = 2\delta_{kk'}$.

The unitary transformation $u_{ij} = \gamma_i + \gamma_j$ interchanges γ_i with γ_j and adds a minus sign to all other operators γ_k with $k \neq i, j$:

$$u_{ij} \gamma_k u_{ij}^\dagger = \begin{cases} \gamma_i & \text{when } k=j, \\ \gamma_j & \text{when } k=i, \\ -\gamma_k & \text{otherwise.} \end{cases} \quad (\text{A4})$$

1. Winding trajectories

We start with the case in which all vortices move along closed trajectories. If m_k is the number of windings of the k th vortex around other vortices, then Ω_k changes by $2\pi m_k$. In view of Eqs. (7) and (8), this implies that the Majorana operator γ_k is multiplied by $(-1)^{m_k}$.

In the simplest case vortex 1 encircles vortex 2, leading to both γ_1 and γ_2 being multiplied by -1 , with all other operators unchanged. This is a consequence of the fact that a phase factor 2π of the order parameter leads to a phase π (and thus a minus sign) for the fermionic operators. In the general case, we need to find a unitary transformation U_{wind} by requiring

$$U_{\text{wind}} \gamma_k U_{\text{wind}}^\dagger = \begin{cases} -\gamma_k & \text{when } m_k \text{ is odd,} \\ \gamma_k & \text{when } m_k \text{ is even.} \end{cases} \quad (\text{A5})$$

This is satisfied by the operator

$$U_{\text{wind}} = \prod_{k=1}^{2N} u_k^{m_k}, \quad (\text{A6})$$

where the operator ordering in U_{wind} is not important up to an overall minus sign.

2. Exchange trajectories

Exchange trajectories in which some of the vortices trade places are more complicated since the phase changes of Ω_k associated with a particular trajectory do not only depend on the winding numbers, but also on the details of the trajectory and on the precise definition of the cut of the function $\arg(\mathbf{r})$ where its value jumps by 2π . The simplest example is the interchange of two vortices. Inevitably one of the vortices crosses the cut line of the other vortex. Thus such an interchange involves an operator u_{12} that exchanges the positions of the two vortices and an operator u_1 or u_2 that multiplies the appropriate vortex by -1 . As a result, the unitary transformations generated by these exchanges are

$$U^{1\rightleftharpoons 2} = \frac{1}{\sqrt{2}}(1 + u_2 u_1), \quad (\text{A7})$$

$$U^{1\rightleftharpoons 2} = \frac{1}{\sqrt{2}}(1 + u_1 u_2). \quad (\text{A8})$$

The transformation $U^{1\rightleftharpoons 2}$ transforms $c_1 \rightarrow c_2$ and $c_2 \rightarrow -c_1$ while $U^{1\rightleftharpoons 2}$ transforms $c_1 \rightarrow -c_2$ and $c_2 \rightarrow c_1$.

The combination of the motion of the first vortex from \mathbf{R}_1 to \mathbf{R}_2 and the motion of the second vortex from \mathbf{R}_2 to \mathbf{R}_1 generates a closed curve. When that curve encloses a third vortex, the phase of that vortex changes by 2π , and so does the phase of one of the first two vortices. Altogether, this gives three phase shifts of 2π , and the transformations $U^{1\rightleftharpoons 2}$ and $U^{1\rightleftharpoons 2}$ have to be multiplied by either $u_3 u_1$ or $u_3 u_2$. There are two possible outcomes to that. The first is $u_3(u_1 + u_2)$, a transformation in which the phase of each of the three vortices is shifted by 2π . The second is $u_3(u_1 - u_2)$, in which the phase of the third vortex is shifted by 2π , and the other two 2π shifts are both given to one vortex.

APPENDIX B: ORTHOGONALITY OF VORTEX STATES

In this appendix, we discuss the scheme to generate the functions $w_i^{(k)}(\mathbf{r})$ in more detail and prove the orthogonality relation (42). We start by proving the orthogonality of the states $w_i^{(0)}(\mathbf{r})$ and $w_j^{(1)}(\mathbf{r})$. In spinor notation, we can write

$$Z_i^{(1)} = i \sum_E \text{sgn } E C_E^i \begin{pmatrix} u_E(\mathbf{r}) \\ v_E(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} w_i^{(1)}(\mathbf{r}) \\ [w_i^{(1)}(\mathbf{r})]^* \end{pmatrix} \quad (\text{B1})$$

in terms of the expansion coefficients

$$C_E^j = \frac{1}{\sqrt{2}} \left\langle \begin{matrix} u_E \\ v_E \end{matrix} \middle| \begin{matrix} i w_j^{(0)} \\ -i [w_j^{(0)}]^* \end{matrix} \right\rangle. \quad (\text{B2})$$

These coefficients satisfy the relation

$$C_{-E}^j = [C_E^j]^* \quad (\text{B3})$$

whose proof uses the identity $u_E(\mathbf{r}) = [v_{-E}(\mathbf{r})]^*$. The states $w_i^{(0)}(\mathbf{r})$ and $w_j^{(1)}(\mathbf{r})$ are obviously orthogonal due to their localization properties for $i \neq j$. For $i = j$, the orthogonality follows from

$$\text{Re} \langle w_i^{(1)} | w_i^{(0)} \rangle = \frac{1}{2} \left\langle \begin{matrix} w_i^{(1)} \\ [w_i^{(1)}]^* \end{matrix} \middle| \begin{matrix} w_i^{(0)} \\ [w_i^{(0)}]^* \end{matrix} \right\rangle = 0 \quad (\text{B4})$$

and

$$\begin{aligned} \text{Im} \langle w_i^{(1)} | w_i^{(0)} \rangle &= -\frac{1}{2} \left\langle \begin{matrix} w_i^{(1)} \\ [w_i^{(1)}]^* \end{matrix} \middle| \begin{matrix} i w_i^{(0)} \\ -i [w_i^{(0)}]^* \end{matrix} \right\rangle \\ &= \frac{i}{2} \sum_E \text{sgn } E |C_E^i|^2 = 0. \end{aligned} \quad (\text{B5})$$

Here, Eq. (B4) uses that by construction, the spinor $Z_i^{(1)}$ has zero overlap with the zero-energy spinors. Equation (B5) uses the symmetry (B3) of the expansion coefficients C_E^i .

We now turn to the higher iterations $w_i^{(k)}(\mathbf{r})$ and proceed to prove the orthogonality Eq. (42). Using the completeness

of the eigenfunctions of the BdG equations, we obtain the useful result

$$S^\dagger S = 1 - \frac{1}{2} \sum_j \left| \begin{matrix} w_j^{(0)} \\ [w_j^{(0)}]^* \end{matrix} \right\rangle \left\langle \begin{matrix} w_j^{(0)} \\ [w_j^{(0)}]^* \end{matrix} \right|, \quad (\text{B6})$$

with S a Hermitian operator $S = S^\dagger$.

For different vortices, $i \neq j$, the orthogonality follows again from the locality properties of the w 's. Thus, we focus on states from the same vortex, $i = j$, and drop the subscript labeling the vortex in the remainder of this appendix. In each iterative step k of the construction of the w 's, we need to prove that

$$\langle w^{(l)} | w^{(k)} \rangle = 0 \quad (\text{B7})$$

for all $l < k$. Since this amounts to a proof by induction, we may exploit that two states w with indices smaller than k are orthogonal.

Starting with $l=0$, we have

$$2\text{Re} \langle w^{(k)} | w^{(0)} \rangle = \left\langle \begin{matrix} w^{(k)} \\ [w^{(k)}]^* \end{matrix} \middle| \begin{matrix} w^{(0)} \\ [w^{(0)}]^* \end{matrix} \right\rangle = 0 \quad (\text{B8})$$

since by construction, the spinor Z_k has zero overlap with zero-energy spinors. Furthermore,

$$\begin{aligned} -2 \text{Im} \langle w^{(k)} | w^{(0)} \rangle &= \left\langle \begin{matrix} w^{(k)} \\ [w^{(k)}]^* \end{matrix} \middle| \begin{matrix} i w^{(0)} \\ -i [w^{(0)}]^* \end{matrix} \right\rangle \\ &= -i \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \sigma_z S \sigma_z \begin{matrix} w^{(0)} \\ [w^{(0)}]^* \end{matrix} \right\rangle \\ &= i \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \sigma_z \begin{matrix} w^{(1)} \\ [w^{(1)}]^* \end{matrix} \right\rangle = 0. \end{aligned} \quad (\text{B9})$$

For $l=1, 2, \dots, k-2$, we obtain

$$\begin{aligned} 2\text{Re} \langle w^{(k)} | w^{(l)} \rangle &= \left\langle \begin{matrix} w^{(k)} \\ [w^{(k)}]^* \end{matrix} \middle| \begin{matrix} w^{(l)} \\ [w^{(l)}]^* \end{matrix} \right\rangle \\ &= \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| (-S \sigma_z)^\dagger (-S \sigma_z) \begin{matrix} w^{(l-1)} \\ [w^{(l-1)}]^* \end{matrix} \right\rangle \\ &= \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \begin{matrix} w^{(l-1)} \\ [w^{(l-1)}]^* \end{matrix} \right\rangle \\ &\quad - \frac{1}{2} \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \sigma_z \begin{matrix} w^{(0)} \\ [w^{(0)}]^* \end{matrix} \right\rangle \\ &\quad \times \left\langle \begin{matrix} w^{(0)} \\ [w^{(0)}]^* \end{matrix} \middle| \sigma_z \begin{matrix} w^{(l-1)} \\ [w^{(l-1)}]^* \end{matrix} \right\rangle = 0 \end{aligned} \quad (\text{B10})$$

and

$$\begin{aligned} -2 \text{Im} \langle w^{(k)} | w^{(l)} \rangle &= \left\langle \begin{matrix} w^{(k)} \\ [w^{(k)}]^* \end{matrix} \middle| \begin{matrix} i w^{(l)} \\ -i [w^{(l)}]^* \end{matrix} \right\rangle \\ &= -i \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \sigma_z S \sigma_z \begin{matrix} w^{(l)} \\ [w^{(l)}]^* \end{matrix} \right\rangle \\ &= i \left\langle \begin{matrix} w^{(k-1)} \\ [w^{(k-1)}]^* \end{matrix} \middle| \sigma_z \begin{matrix} w^{(l+1)} \\ [w^{(l+1)}]^* \end{matrix} \right\rangle \end{aligned}$$

$$= \left\langle \begin{array}{c} w^{(k-1)} \\ [w^{(k-1)}]^* \end{array} \middle| \begin{array}{c} iw^{(l+1)} \\ -i[w^{(l+1)}]^* \end{array} \right\rangle = 0. \quad (\text{B11})$$

Finally, we note for $l=k-1$ that $\text{Re}\langle w^{(k)} | w^{(k-1)} \rangle = 0$ can

be obtained in complete analogy to Eq. (B10) and $\text{Im}\langle w^{(k)} | w^{(k-1)} \rangle = 0$ in analogy with Eq. (B5).²⁴ This completes the iterative construction of the functions $w_j^{(k)}$ including the proof of the orthogonality relations Eq. (42).

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