ZQ topological invariants for Polyacetylene, Kagome and Pyrochlore lattices

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Z_Q Topological Invariants for Polyacetylene, Kagome and Pyrochlore lattices

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Adiabatic Z_Q invariants by quantized Berry phases are defined for gapped electronic systems in d-dimensions ($Q = d + 1$). This series includes Polyacetylene, Kagome and Pyrochlore lattice respectively for $d = 1, 2$ and 3. The invariants are quantum Q-multimer order parameters to characterize the topological phase transitions by the multimerization. This fractional quantization is protected by the global Z_Q equivalence. As for the chiral symmetric case, a topological form of the Z_2-invariant is explicitly given as well.

Introduction: Although the symmetry breaking has been quite successful for a description of phases of matter, recent development in condensed matter physics reveals that there are classes of physically important phases where the symmetry breaking does not play any fundamental roles. Quantum Hall (QH) effects are historical examples. Although there are many apparently different QH states, none of them are characterized by the symmetric properties, where topological quantities, such as, fractional statistics of quasi-particles [1], topological degeneracy[2] and the Chern numbers[3, 4] as the topological invariants are fundamentally important. The topological order is a generic concept for such phases[2] and the geometrical phases based on the Berry connection supply explicit topological order parameters for them [5].

In such topological phases, many of them are gapped and form a class of quantum liquids where the adiabatic invariants play fundamental roles protected by quantization due to the finite gap. They are topological order parameters. Such successful examples are the Chern numbers for the integer QHE[3] and Z_2-Berry phases for the itinerant electrons and gapped quantum spins [5]. Topological insulators (in a restricted sense) for the quantum spin Hall effects as the time-reversal(TR) invariant QHE provide other important examples of the Z_2-quantization[6, 7]. Another fundamental feature of the topological phases is the bulk-edge correspondence[8]. Even if the bulk is featureless, low energy excitations are localized near the boundaries or impurities, which are fundamentally governed by the non trivial bulk.

One of these quantum liquids is a class of the spin liquids for frustrated quantum spins where geometrical frustration and/or quantum fluctuation prevent the system from formation of conventional magnetic order. We have demonstrated the validity of the Z_2-Berry phases where the TR symmetry as the anti-unitary invariance[5, 9] protects their quantization. As for the itinerant electrons with frustration, the same consideration can be applied including spins and orbitals as additional local degrees of freedom. Formation of diagonal order such as magnetism, charge order and orbital order can be suppressed due to the geometrical frustration and/or quantum fluctuation. Then possible stabilization of the quantum states is provided by a dimer formation and its generalization as a multimer formation. To relax a local entropy, quantum mixing among the local degrees of freedom is quite effective to form a local quantum object. It is a multimer in general. In other words, it is a local covalent molecule (with spin). When the total system is composed of weakly interacting such local covalent multimers, it is natural to expect a gapped ground state. We do have such examples experimentally and theoretically[10–12]

Although the covalent molecule as the multimer is simple, it is a purely quantum mechanical object such as the local spin singlet. Then it is natural to characterize the quantum phase by this multimer as the quantum local order parameter. In cases of the spin liquids, the Z_2 Berry phases are quite successful to capture the local singlet [5, 9]. In this work, simple topological expression for this Z_2 Berry phases is explicitly given. Moreover, corresponding to more general symmetries, we provide Z_Q quantization of Berry phases, which are again quite successful to identify the Q-multimer. We demonstrate the validity for a one-dimensional dimer as the model of Polyacetylene, fermions on the Kagome lattice in 2-dimensions and Pyrochlore lattices in 3-dimensions. The Kagome and Pyrochlore systems are canonical frustrated elect on systems and main targets of many experimental and theoretical studies[10, 13–15]. Surprisingly these physically important systems are parts of the generic $Q = (d + 1)$-multimer models in d-dimensions (hyper-Pyrochlore) and discussed in a unified way.

Hyper-Pyrochlore lattice in d-dimensions: Let us provide a hyper-Pyrochlore lattice in d-dimensions. We consider fermions on this lattice at the filing factor $1/Q$ per site, which has a Q-multimerization transition ($Q = d+1$) as the quantum phase transition.

Unit translations of the system are given as

$$e_j = E_j - E_Q,\ j = 1, \cdots, d$$

where $\{E_j, j = 1, \cdots, d + 1 = Q\}$ is a set of equivalent Q points distributed on the d-dimensional sphere $S^d = \{x \big| |x| = 1\}$ those form a hyper-tetrahedron in d-dimensions. $S^0 = \{\pm 1\}$ is a set of 2 points, S^1 is a unit

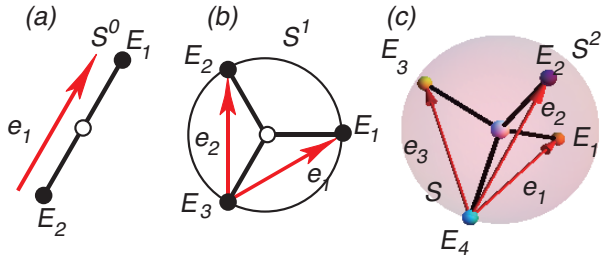

FIG. 1. Vertexes of hyper-tetrahedrons $\{E_j\}$ and unit translations $\{e_j\}$ in d-dimensions. (a): $d=1$, (b): $d=2$ and (c): $d=3$.)

circle and S^2 is a unit sphere (Fig.1) [16]. The set $\{E_j\}$ are two points for $d=1$, vertexes of equilateral triangles in $d=2$ and those of regular tetrahedron in $d=3$. Note that the unit vectors $\{e_j\}$ form unit translations of the generic Creutz hamiltonian in d-dimensions as the generic graphene[17].

The hyper-Pyrochlore lattice is given by the decorating this Creutz model. We put $Q=d+1$ intra sites at the positions $\{-e_j/2\}$ $(j=1,\cdots,d,Q)$ within the unit cell where we define $e_Q=0$. This Q intra sites form (blue) hyper-tetrahedron. These blue hyper-tetrahedrons are connected by the the other (red) hyper-tetrahedrons which can be labeled at the same time as $e_j/2$, $(j=1,\cdots,d,Q)$ (See Fig.2). Here the hyper-tetrahedron in $d=1$ is a pair of sites, that in $d=2$ is an equilateral triangle and it is tetrahedron in $d=3$.

The hamiltonian of the fermions on the hyper-Pyrochlore lattice is given as

$$H=\sum_r t_B[C_B(r)]^\dagger C_B(r)+t_R[C_R(r)]^\dagger C_R(r),\ t_R,t_B\in\mathbb{R}$$

where $C_B(r)=\sum_{j=1}^{d+1}c_j(r)$ and $C_B(r)=\sum_{j=1}^{d+1}c_j(r+e_j)$ with $r=n_1e_1+\cdots+n_de_d$, $(n_j\in\mathbb{Z})$ which is a label of the unit cell. The fermion annihilation operator at the site r of the kind j is denoted by $c_j(r)$. The present hyper-Pyrochlore lattice can be understood as a line graph hamiltonian of the generic Creutz hamiltonian[18]. We consider a case, $t_{B,R}<0$, in this letter. Then the hamiltonian is negative semi-definite, that is, one particle energy is at most zero [19]. In the momentum representation, $c_j(r)=(N_1\cdots N_d)^{-1/2}\sum_k e^{ik\cdot r}c_j(k)$, $(j=1,\cdots,Q)$, $k\cdot r=k_1n_1+\cdots+k_dn_d$ and N_j is a number of unit cells in j-direction, we have $H=\sum_k c^\dagger(k)h(k)c(k)$,

$$h=Q(t_Bp_B+t_Rp_R)=\psi D\psi^\dagger,\quad D=Q\begin{pmatrix}t_B&0\\0&t_R\end{pmatrix}$$

where $c^\dagger(k)=(c_1^\dagger(k),\cdots,c_Q^\dagger(k))$, $\psi_B^\dagger(k)=(1,\cdots,1)/\sqrt{Q}$, $\psi_R^\dagger(k)=(e^{ik_1},\cdots,e^{ik_d},1)/\sqrt{Q}$, and $\psi=(\psi_B,\psi_R)$. The operators $p_B=\psi_B\psi_B^\dagger=p_B^2$, $p_R=\psi_R\psi_R^\dagger=p_R^2$ are projections into the linear space spanned by ψ_B and ψ_R respectively. The states ψ_B and ψ_R are normalized, $\psi_B^\dagger\psi_B=\psi_R^\dagger\psi_R=1$, but generically not orthogonal $\psi_B\psi_R\neq 0$,

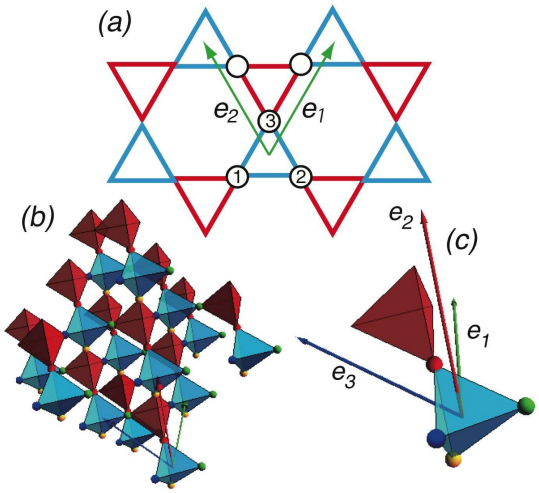

FIG. 2. Unit cells and unit vectors of hyper-Pyrochlore, (a) Kagome lattice ($d=2$), (b), (c) Pyrochlore lattice ($d=3$).

$$\psi^\dagger\psi=\begin{pmatrix}1&\Delta\\\Delta^*&1\end{pmatrix}\equiv\mathcal{O},\quad \Delta(k)=\psi_B^\dagger\psi_R=1+\sum_{j=1}^{d}e^{-ik_j}.$$

Since a linear space is invariant for linear operations, the hamiltonian is diagonalized within the space spanned by ψ_B and ψ_R. Then it is now clear that the hamiltonian $h(k)$ has at most two non zero eigen values and the others are zero. These non zero energy eigen states are spanned by ψ_B and ψ_R [20]. Then the spectrum is composed on the two non trivial bands and the $Q-2$ flat bands at zero energy. In this work, we consider a many body state of the filling factor $1/Q$, that is, the only the lowest band is completely filled.

When the states ψ_B and ψ_R are not linearly independent, which only occurs at the origin $k=0$, one of the two bands touches to the zero mode flat bands ($k=0$ is the only touching momentum). Except this touching momentum, the overlap matrix is regular as $\det\mathcal{O}=1-|\Delta|^2\neq 0$.

Projecting out the zero modes, the hamiltonian for the non zero energy bands is diagonalized by a linear combination of ψ_B and ψ_R. Then the Schrodinger equation reduces to the following generic secular equation $\mathcal{O}D\mathcal{O}\phi=E\mathcal{O}\phi$ where $\phi={}^t(\phi_B,\phi_R)$ is a two dimensional vector. The two band energies are given by the eigen values of $h_\psi=\mathcal{O}^{1/2}D\mathcal{O}^{1/2}$ assuming $\det\mathcal{O}\neq 0$. Then noting that $\det h_\psi=\det D\det\mathcal{O}=Q^2t_Bt_R\det\mathcal{O}$ and $\mathrm{Tr}\,h_\psi=\mathrm{Tr}\,h=Qt_B\mathrm{Tr}\,p_B+Qt_R\mathrm{Tr}\,p_R=Q(t_B+t_R)$, the non trivial two band energies are given by

$$E(k)=(Q/2)\big(t_B+t_R\pm\sqrt{(t_B-t_R)^2+t_Bt_R|\Delta(k)|^2}\big)$$

which is the energy dispersion of the hyper-Pyrochlore system. When the two bands are degenerate, the Dirac fermions appear and the many body state with the filling $1/Q$ state becomes critical, which occurs only when

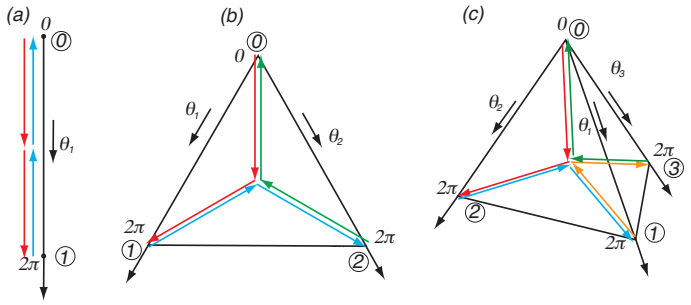

FIG. 3. $Q = d + 1$ paths $L_1, \cdots, L_Q$ to define Z_Q Berry phases in the parameter space T^d.

$t_B = t_R$. This is a quantum critical point of the Q-multimerization transition. We have two different Q-multimerization phases, which are gapped ground states both for $t_B < t_R$ and $t_B > t_R$. In the following, we give topological order parameters for this quantum phase transition using Z_Q adiabatic invariants as Berry phases.

Before describing the construction of the topological order parameter, let us discuss zero modes of generic multimer system in real space. Consider a hamiltonian $H = \sum_\alpha t_\alpha C_\alpha^\dagger C_\alpha$, $t_\alpha \in \mathbb{R}$, where $C_\alpha = (\xi_1 c_{\alpha_1} + \cdots + \xi_{\alpha_{N_\alpha}} c_{\alpha_{N_\alpha}}) = \psi_\alpha c$ is a annihilation operator of an N_α-multimer, $c^\dagger = ({c_1}^\dagger, \cdots)$ where α is a label of the generic N_α-multimer in real space. Then ψ_α is a normalized multiplet, which is the molecular orbital of the N_α-multimer as $\psi_\alpha^\dagger \psi_\alpha = |\xi_1|^2 + \cdots + |\xi_{N_\alpha}|^2 = 1$. Note that the lattice structure is arbitrary. Since the hamiltonian is again given by a sum of projections as $H = c^\dagger \big[\sum_\alpha t_\alpha p_\alpha\big] c$ where $p_\alpha = \psi_\alpha \psi_\alpha^\dagger$, the discussion above is directly applied[20]. Then the number of zero modes, N_Z is, at least, given by $N_Z^{\min}$

$$N_Z \geq N_Z^{\min} \equiv \#(\text{sites}) - \#(\text{molecular orbitals})$$

Z_Q Berry phases: Let us define a Berry phase introducing a d-dimensional parameters $\Theta = (\theta_1, \cdots, \theta_d)$ where θ_j is defined on mod 2π, that is, Θ is define on the torus $\Theta \in T^d$. It modifies a local blue hyper-tetrahedron only at r as

$$C_B(r) \to C'_B(r) = \sum_{j=1}^{Q=d+1} e^{i\varphi_j} c_j(r)$$

where $\varphi_j = \sum_{i=1}^j \theta_i$, $(j = 1, \cdots, d)$ and $\varphi_Q = 0$. If this hyper-tetrahedron is decoupled from the other ($t_R = 0$), it is a gauge transformation. However, it is not the case and the phases are not gauged away generically. Using a loop (closed paths) L_j, $(j = 1 \cdots, d)$ on the torus T^d defined below, Berry phases γ_j's are defined as $\gamma_j = -i \int_{L_j} A$, $A = \langle \Psi(\Theta) | d\Psi(\Theta) \rangle$ where $|\Psi(\Theta)\rangle$ is a many body state which are energetically well separated from the above for ${}^\forall\Theta$. The loop L_j is defined as

$$L_j = \ell_j - \ell_{j+1}, \ (\ell_{Q+1} = \ell_1), \quad \ell_j = V_j \to C_G$$

where $V_j = 2\pi e_j$. We use the same e_j to save symbols. It is in the parameter space Θ and not in the real space. This V_j is the j-th vertex of the generic hyper-tetrahedron in the parameter space. The bond length of the hyper-tetrahedron in the parameter space is 2π and C_G is a center of gravity of the hyper-tetrahedron, $C_G = \sum_{j=1}^Q V_j/Q$ (See Fig.3). The hamiltonian on this loop, $H(L_j)$, is periodic. The corresponding Berry phase is well defined as far as the gap remains open.

We note here symmetric properties of the hyper-Pyrochlore system. Single hyper-tetrahedron is invariant for any change of the vertexes S_Q then the hyper-tetrahedron system has this global S_Q symmetry, since the S_Q induces a change of the bases $\{e_j\} \to \{\pm e_{j'}\}$. By the introduction of the phases φ_j, this symmetry is generically broken but we still has a following global Z_Q equivalence defined as

$$H(L_j) = U_Q H(L_{j+1}) U_Q^\dagger, \quad (U_Q)^Q = 1$$

where U_Q is a parameter independent global unitary operator. It operates for the hyper-tetrahedron at r as $U_Q c_{j+1}(r) U_Q^\dagger = c_j(r)$, $c_{Q+1}(r) \equiv c_1(r)$. It implies the Z_Q equivalent of the corresponding Berry phases as

$$\gamma_1 \equiv \gamma_2 \equiv \cdots \equiv \gamma_Q \equiv \gamma, \quad \mod 2\pi$$

where note that the Berry phase is generically gauge dependent and only well defined in modulo 2π [5]. Then noting that a sum of the loop is equal to the zero loop, $\sum_{j=1}^Q L_j \equiv 0$, we have $\sum_{j=1}^Q \gamma_j \equiv Q\gamma \equiv 0$, $(\mod 2\pi)$. It implies Z_Q quantization of the Berry phase as

$$\gamma \equiv 2\pi \frac{n}{Q} \mod 2\pi, \quad n \in \mathbb{Z}$$

Since the quantization of the Berry phases is established, these Berry phases are adiabatic invariants, that is, they never change unless the energy gap closes. When the hopping t_B is sufficiently weak, the res ponce of the ground state against for the modification by θ_j's is very weak, that is, the Berry phases vanish due to the quantization, $\gamma \equiv 0 \ (\mod 2\pi)$. On the other hand, t_B is strong enough compared with t_R, say, $t_R = 0$, the Berry phases are determined by a single hyper-tetrahedron at r. In this case, the change of the θ_j's is given by the gauge transformation of the hamiltonian as[21] $H(L_j) = \mathcal{U}(\Theta) H(0) \mathcal{U}(\Theta)^\dagger$, $\mathcal{U}(\Theta) = \prod_{j=1}^d e^{-i\varphi_j n_j(r)}$, $|\Psi(\Theta)\rangle = \mathcal{U}(\theta)|\Psi(0)\rangle$, $A = -i\langle\Psi(0)| \sum_{j=1}^d n_j(r) |\Psi(0)\rangle d\varphi_j = -i\frac{1}{Q}\sum_{j=1}^d d\varphi_j$ where $n_j(r) = c_j(r)^\dagger c_j(r)$ is a occupation operator at the site j of the hyper-tetrahedron at r. Note that the expectation values are $\langle\Psi(0)|n_j(r)|\Psi(0)\rangle = 1/Q$ due to the Z_Q symmetry of the system without twist Θ. Then the Berry phases along the loop L_j is given as $\gamma = -2\pi\frac{d}{Q} \equiv 2\pi\frac{1}{Q}$, $(\mod 2\pi)$ in the strong coupling limit. It is numerically confirmed as in the Fig.4 for the various hyper-Pyrochlore systems with periodic boundary conditions. The key idea of the Q-multimerization is that the Z_Q equivalence of the Q loops in the hamiltonian manifold and the sum

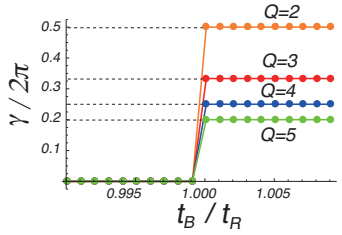

FIG. 4. Numerical calculation of the Berry phases for hyper-Pyrochlore lattices $Q = 2(d = 1)$: $N = 2\cdot 200^1$, $Q = 3(d = 2)$: $N = 3\cdot 14^2$, $Q = 4(d = 3)$: $N = 4\cdot 6^3$, $Q = 5(d = 4)$: $N = 5\cdot 4^4$ as a function of the multimerization strength t_B/t_R. The systems are periodic.

of them is equivalent to a zero loop $\sum_j L_j = 0$. These two conditions are satisfied for hyper-Pyrochlore systems constructed with the parameter Θ in any dimension.

Z_2-invariant for a Chiral symmetric system: Our hyper-Pyrochlore system for the $Q = 2$ case and the d-dimensional Creutz hamiltonians are reduced into the chiral symmetric system since the diagonal terms in the hamiltonian do not modify the one particle states at all. Generically speaking, the Z_2-equivalence is derived only by the chiral symmetry[22]. In this case, we have a direct and explicit form of the adiabatic Z_2 invariant. The chiral symmetry implies that the hamiltonian, $H = c^\dagger hc$ satisfies $\{h, \Gamma\} = 0$, $\Gamma^2 = I_N$. Then taking a form $\Gamma = \mathrm{diag}(I_{N/2}, -I_{N/2})$, the hamiltonian is written as $h = \begin{pmatrix} & q \\ q^\dagger & \end{pmatrix}$. Then the half filled ground state $|\Psi\rangle$ is given by filling all of the negative energy states as $|\Psi\rangle = (c^\dagger\Psi_1)\cdots(c^\dagger\Psi_N)|0\rangle$, $h\Psi_j = -\epsilon_j\Psi_j$, $(\epsilon_j < 0)$ since $\Gamma\psi_j$ is an eigen state with the energy $\epsilon_j > 0$. We take the one particle states are orthonormalized as $\Psi_i^\dagger\Psi_j = \delta_{ij}$. Here we assume the half filled many body state is gapped. In this case, the Berry connection of the many body state is given as $A = \langle\Psi|d\Psi\rangle = \mathrm{Tr}\, a$ where $a = \Psi^\dagger d\Psi$ is a non-Abelian Berry connection of dimension $N/2$ which is composed of the one particle states as $\Psi = (\Psi_1, \cdots, \Psi_{N/2})$. Writing this normalized multiplet as $\Psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}/\sqrt{2}$, the orthogonality of the states among the different energies implies $\Psi^\dagger\Gamma\Psi = 0$. It reduces to $\psi_A^\dagger\psi_A = \psi_B^\dagger\psi_B = I_{N/2}$ using the normalization of Ψ. Then we also have $\psi_A\psi_A^\dagger = \psi_B\psi_B^\dagger = I_{N/2}$ since $\psi_{A,B}$ are $(N/2)$-dimensional square matrices. Using the Schrodinger equation, $h\Psi = \Psi D$, we have $\psi_B = q^{-1}\psi_A D$. By the projection, $P = \Psi\Psi^\dagger$ and taking a multiplet $\Phi = \begin{pmatrix} I_{N/2} \\ O \end{pmatrix}$ ($\mathcal{O}$ is a $N/2$-dimensional square zero matrix), the gauge fixed normalized multiplet is given as $\Psi_\Phi = P\Phi(\Phi^\dagger P\Phi)^{-1/2} = \begin{pmatrix} I_{N/2} \\ \xi \end{pmatrix}/\sqrt{2}$ where $\xi = q^{-1}g$ and $g = \psi_A D^{-1}\psi_A^\dagger = g^\dagger$. Then the gauge fixed Berry connection a_Φ is explicitly evaluated as $a_\Phi = \Psi_\Phi^\dagger d\Psi_\Phi = \xi^\dagger d\xi/2 = \xi^{-1}d\xi/2$. It gives the Berry phase γ for a closed loop L as

$$\gamma = -\frac{i}{2}\int_L \mathrm{Tr}\,\xi^{-1}d\xi = -\frac{1}{2}\int_L d\,\mathrm{Arg}\det q$$

since g is hermite. It gives an explicit topological expression of the Z_2-Berry phase by the winding number, which gives π when $\det q$ goes around the origin odd number of times in the complex plane. Otherwise it is zero.

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