Quantized Berry Phases as Local Order Parameters of Quantum Liquids

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We propose to use quantized Berry phases as local order parameters of gapped quantum liquids, which are invariant under some anti-unitary operation. After presenting a general prescription, the scheme is applied for Heisenberg models with frustrations and two dimensional extended Su-Schriefffer-Heeger models associated with a random dimer covering. In each phases, the quantized Berry phases, as 0 or π, describe the ground state texture pattern of local singlet bonds and dimer bonds. Also possible applications to large classes of correlated electron systems are discussed.

One of the challenges in modern condensed matter physics is to have well understanding of quantum liquids which do not have classical analogues. States of matters in classical systems are mostly described by the local order parameters based on a concept of symmetry breaking. However, recent studies in decades have revealed many of interesting quantum phenomena are not well characterized by the classical local order parameters, such as quantum Hall effects, exotic superconductors[1] and frustrated or doped quantum magnets[2][3][4]. Quantum spins with $S = 1/2$ and fermions can be objects in quantum limits which do not have classical counterparts. When they get together, one may find some classical degree of the freedom to describe the states approximately. However, it is not always the case. A pair of $S = 1/2$ spins with exchange interaction forms a singlet and a triplet. The latter has a classical analogue as a small magnet, however, the singlet does not. When the total system is composed of such singlet pairs, the system is also in the quantum limit as a singlet spin liquid. The most famous singlet spin liquid can be the RVB state proposed by Anderson as a possible basic platform of the high-temperature superconductors[5]. Quantum spins with $S = 1/2$ and fermions can be objects in quantum limits which do not have classical counterparts. When they get together, one may find some classical degree of the freedom to describe the states approximately. However, it is not always the case. A pair of $S = 1/2$ spins with exchange interaction forms a singlet and a triplet. The latter has a classical analogue as a small magnet, however, the singlet does not. When the total system is composed of such singlet pairs, the system is also in the quantum limit as a singlet spin liquid. The most famous singlet spin liquid can be the RVB state proposed by Anderson as a possible basic platform of the high-$T_c$ superconductors. Also the valence bond solid (VBS) state and the Haldane phases of integer Heisenberg spin chains are the quantum spin liquids of this class[5][6][7]. The ground state of a half filled Kondo lattice also belongs to it, which is a superposition of singlet pairs between the conduction electrons and the localized spins[7]. Some of the dimer models and spins with a string net condensation can be solvable limits of such quantum liquids[8][9][10]. As for a fermion pair, when the hybridization between them is assumed secondary, one may use a classical number basis for the description. However, the picture breaks down in the strong coupling limit, where the state is labeled as bonding or anti-bonding states. They are purely quantum variables, as bonds, that live on the link between the fermions sites. This state with the dimerized fermion pairs can be also understood as a typical quantum liquid.

In these quantum liquids, the classical local order parameter is not enough to characterize the state. We proposed to use generalized topological numbers such as the Chern numbers for the global characterization based on a concept of topological orders[11][12]. Also non local objects such as entanglement entropies can help to capture some of the features[13]. Here we propose to use Berry phases to characterize the quantum liquids locally. The Berry phase is gauge dependent and is not quantized generically[14]. We clarify the gauge dependence and present a prescription to define quantized Berry phases as quantum local order parameters for anti-unitary invariant states. This requirement for the invariance can be complementary to the one for the Chern number description where the time-reversal symmetric states are mostly classified by vanishing topological integers.

Berry phases with Gauge Fixing: Let us first present a prescription to calculate Berry phases for a multiplet which is a generalization of a single eigen state to an eigen space with dimension $D \geq 1$[12]. The multiplet naturally appears in a discussion with degeneracy and is also quite useful to handle a single many body state of the Slater state. (See later). Let us consider a parameter $x$-dependent hermitian hamiltonian which is diagonalized by ortho-normalized eigen states with energies $E_j(x)$ as $H(x)|\psi(x)\rangle = \psi(x)E(x)$, $\psi(x) = (|\psi_1(x)\rangle, \ldots, |\psi_D(x)\rangle)$, $\psi^d_i = 1\delta_{ij}E_j(x)$. We further assume the gap opening condition, $E_1(x) \neq E_k(x)$, $j = 1, \ldots, D$, $k = D + 1, \ldots$, which guarantees a regularity of the multiplet as for $x \in [12]$. A matrix valued Berry connection, $A = \psi^d_i d\psi$ and a closed loop $C$ in the parameter space define the Berry phase, which is customarily written as $i\gamma_C(A) = \int_C Tr A \cdot \omega$. Changing a basis for the multiplet, the multiplet is transformed by a unitary matrix $\Psi = \psi^d \omega$. It induces a gauge transformation $A = \omega^d A \omega + \omega^d d\omega$. The Berry phase, $\gamma_C$, is gauge dependent and thus is not well defined without a specific gauge fixing. Following a general procedure[12], the gauge can be fixed by a multiplet $\Phi$ which is arbitrary and single-valued but not necessarily constant. We define an unnormalized multiplet, $\Psi = P \Phi$ by the gauge invariant projection $P = \psi^d \psi$. It is only normalized as $\Psi_\Phi = \psi^d N_\Phi^{-1/2}$ with the gauge independent requirement $\det N_\Phi \neq 0$ where $N_\Phi = (\Psi^d \psi)^{-1} \psi^d \psi = \eta_\Phi \eta_\Phi^d$, $\eta_\Phi = \psi^d \Phi$ and $\det N_\Phi = |\det \eta_\Phi|^2$. When it is satisfied everywhere on a curve $C$, we call the gauge by the $\Phi$ is regular. Taking the other regular gauge by the multiplet $\Phi'$, the transformation matrix is explicitly given as $\omega = (\Psi_{\Phi'})^{-1} \psi = N^{-1/2}_{\Phi'}(\eta_{\Phi'})^{-1} \eta_\Phi N^{-1/2}_{\Phi'}$ which is
also regular on the loop \( C \). The Berry phase gets modified as \( \gamma_C(A_ϕ) = γ_C(A_ϕ) + Δ(C, ω), Δ(C, ω) = \int_C dArg det_D ω = \int_C dArg det_D η_ϕ/ det_D η_ϕ \). Since the overlap matrices \( η_ϕ, \Phi_ϕ \) are single-valued and regular on the \( C \), we have \( Δ(C, ω) = 2πMC \) with some integer \( MC \). (Generically we expect \( MC = 1 \), but one may have \( MC > 1 \) with some additional symmetry.) It implies that the Berry phase in a regular gauge (regular Berry phase) has a gauge invariant mapping up to this integer as \( γ_C = -i MC \). This is topological since small perturbations can not modify the Berry phase unless the gauge becomes singular.

Anti-Unitary Symmetry and Quantized Berry phases: Now let us consider a parameter independent discrete symmetry described by an anti-unitary operator \( Θ = KU_0 \) where \( K \) is a complex conjugation and \( U_0 \) is unitary. It operates for a state expanded by a parameter \( x \).

It is invariant under the anti-unitary operation \( \{ H, Θ \} = 0 \). When the eigen state \( | G \rangle \) is unique, \( | G \rangle \) and \( | G_Θ \rangle \) are different just in their phases (gauges). They span the same (one dimensional) linear space. With the generic argument before, it implies \( \gamma_C(G) ≡ γ_C(G_Θ) \). To be compatible with the transformation property with \( Θ \), the Berry phase of the anti-unitary invariant state is inevitably quantized as \( \gamma_C(G) = 0, πMC \). We just assume a anti-unitary symmetry, \( Θ \). It operates for a state expanded by a parameter \( x \).

We propose to use the quantized Berry phases to define a local topological order. Let us consider a quantum many body state \( | G \rangle \) which is an eigen state of a hamiltonian \( H \). We do not require a translational symmetry and the system may have boundaries as well. We just assume an anti-unitary invariance of the hamiltonian by the operator \( Θ \). Further we assume that the (ground) state is gapped and unique, i.e., it is invariant under the anti-unitary operation. Then introducing a local perturbation at \( r \) specified by a set of parameters \( x_r \), we define a hamiltonian \( H(x_r) \) which preserves the symmetry requirement as \( \{ H(x_r), Θ \} = 0 \). Taking some close curve \( C_r \) in the parameter space, we have two possibilities: (a) \( | G \rangle \) is unique \( \forall x_r \in C_r \) or (b) \( | G \rangle \) is degenerate at \( x_r \in C_r \).

In the first case, we identify the quantized Berry phase \( γ(C_r) \) as the local order parameter at \( r \). We expect that the degeneracy occurs as in the latter case, it implies gapless localized excitations (edge states) are induced by the perturbation \( \sum_r \). In a fermion bilinear hamiltonian system, it is an appearance of localized zero modes. This also characterizes the location \( r \) of the quantum state \( | G \rangle \). Then we assign one of the three labels, \( \{ πMC \}, \{ 0 \} \) to the position \( r \). We propose to use them as local topological order parameters for the gapped quantum liquid.

To evaluate the quantized Berry phase for some specific models numerically, one needs to specify the gauge and discretize the loop \( C \) as \( x_0, x_1, \ldots, x_N = x_0 \). Then we define a lattice Berry phase \( γ_C^N(A_ϕ) \) by the lattice Berry connection \( \sum_{j=1}^N \). In the large \( N \) limit, it reduced to the standard one. A generic choice of the multiplet \( Φ \) is expected to induce a regular gauge. In the numerical calculations below, we take random vectors for them.

**Heisenberg Models on a Frustrated Lattice**: We apply the generic formulation here for specific models. The first example is a generic Heisenberg model on any lattice in any dimensions. We allow frustrations among spins. The hamiltonian is given as \( H^{sp} = \sum_{ij} J_{ij} S_i \cdot S_j \) where \( \{ S_i \} \sim \{ S_{ix}, S_{iy}, S_{iz} \}, S_{ix} = \frac{1}{2} I_{xα}, α = x, y, z \) and \( S_α ' s \) are the Pauli matrices. A time-reversal operator, \( Θ_T = K \otimes \otimes (iσ_y) \), is used to describe the anti-unitary symmetry. It operates for a generic spin state \( | G \rangle = \sum C_j|σ_1, σ_2, \ldots, σ_N \rangle \), \( | σ_i = ±1 \rangle \) as \( Θ_T|G \rangle = \sum C_j(-)^{\sum_{i=1}^N(1+σ_i)/2} |σ_1, \ldots, σ_N \rangle \). The spins get

**FIG. 1**: A flux loop as a local probe to define quantized Berry phases for picking up a local topological order. (a) Schematic figure. (b) A local gauge to define the flux loop.
transformed as $S_j \rightarrow \Theta^{-1}_j S_j \Theta = -S_j$. It is
due that the Hamiltonian is invariant as $\Theta^{-1}_j H \Theta = H$. A
local perturbation to define the quantized Berry
phase is constructed by a local gauge transformation $S_j \rightarrow S'_j(\varphi_j) = e^{i\varphi_j} n^\dagger_j S_j e^{-i\varphi_j} n_j = Q_j(\varphi) S_j$ where
$Q(\varphi) = e^{i\varphi} T$ is a real $3 \times 3$ matrix and the $T$ is real
skew-symmetric as $T^{\alpha\beta} = 4i n^\dagger_j S^\alpha_j S^\beta_j$. We take $n = (0, 0, 1)$ without losing a
generality. Then the local hamiltonian is written in the
transformed basis as $J_{ij} S_i \cdot S_j = h_{ij}(S'_i, S'_j, \theta_{ij}) = \frac{1}{2}(e^{-i\theta_{ij}} S_{ij}' + e^{i\theta_{ij}} S_{ij}'^\dagger) + S_{ij}' S_{ij}'$ where
$\theta_{ij} = \varphi_i - \varphi_j$. Based on the observation, let us con-
sider a Heisenberg model with a local perturbation at the
link $\langle i,j \rangle$ as $H^{sp} = e^{i\theta}(\sum_{ij} h_{ij}(S_i, S_j, \theta_{ij}), \text{ where } \theta_{ij} = \theta \text{ for } \langle ij \rangle = \langle i,j \rangle \text{ and } 0 \text{ otherwise.}$ Then
consider a quantized Berry phase $\gamma_{ij}^{sp}$ by the unit cir-
cle $C$. Note that this local twist is not gauget away
globally and induces a local perturbation which preserves
the time-reversal symmetry. Let us first consider a special
configuration of the interactions $J_{ij}$. Taking any
nearest-neighbor dimer covering of all sites $D = \{(ij)\}$
($|D| = N/2$, $N$ is a number of total sites), we as-
ume that the interaction is nonzero only on these dimer
links as $H^{sp} = \sum_{\langle ij \rangle \in D} J_{ij} S_i \cdot S_j$ ($\forall J_{ij} > 0$). The
ground state $|G\rangle$ is unique and gapped. It is also in-
vARIANT as for the time-reversal operation. When the
link $\langle i,j \rangle$ does not belong to the dimer covering $D$, the
Berry phase is approximately vanishes $\gamma_{ij}^{sp} = 0$. When
the dimer covering includes the link $\langle i,j \rangle$, the
ground state in the regular gauge is explicitly given as
$|G_{\varphi}\rangle = |i,j\rangle \Psi_{\varphi}(e^{i\varphi}) \otimes \delta_{\langle ij \rangle \neq \langle i,j \rangle} |(ij)\rangle \Psi_{\Phi}(1)$ where
$|ij\rangle = (|+\rangle i f -|j\rangle f -|j\rangle f -|+\rangle i f)$. Then the quantized Berry
phase is evaluated as similar to the example $(H^D)$. It is
clear that the quantized Berry phases pick up the dimer
pattern $D$ as $\gamma_{ij}^{sp} = \pi : (ij) \in D$ and $\gamma_{ij}^{sp} = 0 : (ij) \notin D$. Now let us imagine an adiabatic process to include
interactions across the dimers. Due to the topological
stability of the quantized Berry phase, they can not be
modified unless the dimer gap collapses. This dimer limit
presents a non-trivial example and shows the usefulness
of the quantized Berry phases as local order parameters
of singlet pairs. To show its real validity of the quanti-
zied Berry phases, we have diagonalized the Heisenberg
hamiltonians numerically by the Lanczos algorithm and
calculated $\gamma_{C_{ij}}^{sp}$ numerically. Some of the results are
shown in Fig. 2 as a demonstration. Clearly the quanti-
zied Berry phases are quite powerful to describe texture
patterns of the singlet liquid phase.

**Dimerization of Spinless fermions and the Slater States:** Another example of the anti-unitary operator is a
particle-hole symmetry operation for fermion systems.
To be specific let us discuss a spinless fermion with a
particle-particle interaction by a hamiltonian $H^{sl}(x) = \sum_{\langle ij \rangle} t_{ij}(x)c^\dagger_i c_j + t_{ij}^\dagger(x)c^\dagger_j c_i + V_{ij}(x)(n_i - \frac{1}{2})(n_j - \frac{1}{2})$, where $c_i$ is a fermion annihilation operator. We divide $N$ lattice
sites into $A$ and $B$ sublattices. The particle-hole conjugation operator, $\Theta_P$, which is anti-unitary is defined by

$\Theta_P = KU_P$, $U_P = \prod_{j=1}^N e^{i\xi_j \sigma_z + \xi_j' \sigma_x}$, $\xi_j, \xi_j' \in A \in B$, $\xi_j, \xi_j' \in B$ where $\xi_j = (c_j + c_j^\dagger) \text{ and } \xi_j' = (c^\dagger_j - c_j)$. When the lattice is bipartite
and the hopping $t_{ij}$ connects sites between the sublattices $A$ and $B$, the hamiltonian is anti-unitary invariant by
$\Theta_P$ as $\Theta_P H^{sl}(x) \Theta_P = H^{sl}(x)$. Thus a generic $M$-particle
state, $|G_{N}\rangle$ is degenerate with the $(N-M)$-particle state,$|G_{N-M}\rangle = \Theta_P |G_N\rangle$. It implies that the eigen space of the
$\Theta_P$ operator is not one-dimensional except the half
filled case $(N = 2M)$. In this half filled case, we apply the
present characterization by the quantized Berry phase
assuming the state is unique and gapped. We take a local
perturbation at a link $(i,j)$ similarly to the Heisenberg
spins as $t_{ij} = t(|i\rangle|j\rangle e^{i\theta_{ij}}$, where $\theta_{ij} = \theta$ for $(i,j) = \langle i,j \rangle$ and $0$ otherwise. Taking a unit circle $C$, the quantized
Berry phase is evaluated. We have performed exact di-
egonalizations similar to the Heisenberg spins. How-
ever, we show here further analysis assuming the
system is non-interacting $V_{ij} = 0$. When we assume that
the hopping is only non zero among the dimers in some
dimer covering $D$, the quantized Berry phases repro-
duce the dimer pattern. This model can be understood
as a generalization of the Su-Schrieffer-Heeger (SSH)
model in one-dimension. In the dimer limit, the
particle-hole symmetric unique ground state is given as
$|G_{\varphi}\rangle = [c^\dagger_{(i,j)} \Psi_{\varphi}(e^{i\varphi}) \prod_{\langle ij \rangle \neq \langle i,j \rangle} [c^\dagger_j \Psi_{\Phi}(1)] |0\rangle$ where
c^\dagger_j = (c^\dagger_j, c_j^\dagger)$. The regular Berry phase is then evaluated as
$\gamma_{C_{ij}}^{sp} (|G_{\varphi}\rangle) = \pi : (ij) \in D, 0 :$ (otherwise). Due to the
topological stability, this texture pattern is only modified
after a quantum phase transition. The quantized Berry
phases here play a role of topological order parameters of
the local dimerization.

In this non-interacting case, the non-Abelian formulation
here is quite useful for the evaluation of the Berry

![FIG. 2: A distribution of π-bonds for frustrated Heisenberg models on a 4 × 4 lattice with periodic boundary condition. The most thick lines denote the π-bonds. The other links are 0-bonds. (a) Next-Nearest-Neighbor exchanges are $J_N^{NN} = 0.5$, nearest neighbor exchanges are $J_N^{NN} = 2$ or $J_N^{NN} = 1$. The links with $J_N^{NN} = 2$ coincide with the π-bonds denoted by the thick lines. (b) Some of the $J_N^{NN}$’s are enhanced from 0.5 to 4. The other are the same as (a). The strong NNN links $J_N^{NN} = 4$ coincide with the π-links. Dimerized links, $J_N^{NN} = 2$, (the same as (a)) are shown as gray lines, which are 0-bonds in this phase. (They are π-bonds in (a).)
phase of a single many body state. The $M$-particle eigen state (Slater state) is constructed from a set of the one-particle states as (a generic fermi sea) $|G_M\rangle = \prod_{i=1}^M |c^\dagger_i(\varphi)\rangle|0\rangle$, $c^\dagger_i = (c^\dagger_1, \ldots, c^\dagger_N)$, where $|0\rangle$ is a vacuum $\varphi_i, c_i^\dagger = 0$. The ortho-normalized one-particle state $\varphi^\dagger, (\varphi^\dagger, \varphi^\dagger) = \delta_{\ell\ell'}$ is an eigen state of the one-particle hamiltonian $h$ where $h\varphi_i = c^\dagger \epsilon c_i + c^\dagger \hbar \Omega = H^M, (V_{ij} = 0)$. As for this $M$-particle state, a multiplet with a dimension $D=M, \varphi = (\varphi_1, \ldots, \varphi_M)$ defines a non-Abelian Berry connection $A_M = \varphi^\dagger d\varphi$, which gives the Berry connection of the single many-body state $|G_M\rangle$ as $A = (G_M|dG_M) = \text{Tr} A_M$ [22]. It enables us to perform calculations of the Berry phases for quite large systems where the non-Abelian gauge fixing is crucial.

We have demonstrated its validity for an extended SSH model in two dimensions on a $10 \times 10$ periodic lattice as shown in Fig. $3$. The $\pi$-bonds pick up the dimer pattern of the model in the dimer limit and also captured topological structure of the complicated quantum liquid after several quantum phase transitions.

The $tJUV$ model and the Kondo lattice: The present generic scheme can be useful for large classes of correlated electron systems. For example, following $tJUV$ models with Kondo coupling in $d$ dimensions are worthy to be investigated by the scheme, $H^{tJUVK}(x) = \sum_{ij}(H^G_{ij} + H^V_{ij} + H^I_{ij}) + \sum_i (H^U_i + H^K_i), H^G_{ij}(x) = c^\dagger_i t_{ij}(x)c_j + h.c., H^V_{ij} = (n_{ij} - 1)V_{ij}(n_{ij} - 1), H^U_i(x) = s_i J^i_{ij}(x)s_j, H^K_i = U(n_{ij} - 1/2)(n_{ij} - 1/2) = -U^2 s_i^2, H^K_i(x) = \epsilon_i s_i J^K_i(x)S_i$ and $J^i_{ij}(x) = J^{i,\ell}_i = Q(\theta_{ij}^{J,K})(1,1,\lambda^{J,K}_{ij})$, where $c^\dagger_i = (c^\dagger_{1,1}, \ldots, c^\dagger_{n,1})$, $s_i = \frac{1}{2}\epsilon_i \sigma c_i$ and $\epsilon_i = (s_{ix}, s_{iy}, s_{iz})$. In the model, two kinds of anti-unitary operators, the particle-hole conjugation $\Theta_P$ and the time-reversal operation $\Theta_T$ can be the symmetric operations. They are explicitly defined as $\Theta_P = KU_P, U_P = U_P^\dagger U_P, U_P = \prod \epsilon_{ij}\sigma_{ij}$ and $\Theta_T = K \prod e^{i\sigma_{ij}}(s_{ix}, -s_{iy}, s_{iz})$. By these anti-unitary operations, we can consider two different type of local perturbations as discussed. Then the quantized Berry phases are defined as two different local topological order parameters. They can be useful to describe and characterize quantum liquids phases of the correlated electron systems. [20] The ground state of the half filled Kondo lattice is expected to give a non trivial example. At least, in the strong coupling limit, the Kondo coupling links can be labeled as $\pi$-bonds as for the time-reversal symmetry.

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![FIG. 3: Non interacting spinless fermions with hopping modulations, $|t_{ij}| = t_S \text{ or } t_W (\leq t_S)$. The strong links $t_S$ are distributed on a (random) dimer covering configuration. The black thick lines are the strong links with $\gamma = \pi$. The gray thick lines are the strong lines with $\gamma = 0$. The black thin lines are the weak links with $\gamma = \pi$. The other nearest neighbors, which are not drawn, are weak links with $\gamma = 0$. (a) $t_W = 0.6 t_S$ and (b) $t_W = 0.7 t_S$. The dimer configuration is the same. There occur several quantum phase transitions supplemented with gap closings between $t_W : 0.6 \rightarrow 0.7$.](image-url)