Berry phases in superconducting transitions

A.A. Aligia

Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 S.C. de Bariloche, Argentina.

(Received March 24, 2022)

I generalize the concept of Berry’s geometrical phase for quasicyclic Hamiltonians to the case in which the ground state evolves adiabatically to an excited state after one cycle, but returns to the ground state after an integer number of cycles. This allows to extend the charge Berry phase $\gamma_c$ related to the macroscopic polarization, to many-body systems with fractional number of particles per site. Under certain conditions, $\gamma_c$ and the spin Berry phase $\gamma_s$ jump at $\pi$ at the boundary of superconducting phases. In the extended Hubbard chain with on-site attraction $U$ and nearest-neighbor interaction $V$ at quarter filling, the transitions detected agree very well with exact results in two limits solved by the Bethe ansatz, and with previous numerical studies. In chains with spin SU(2) symmetry, $\gamma_s$ jumps when a spin gap opens.

PACS. 03.65 - Quantum theory; quantum mechanics.
PACS. 71.10 - General theories and computational techniques.
PACS. 74.20-z - Theories and models of superconducting state.

In the last decade, Berry phases have caused a great deal of interest in a variety of fields in physics. Applications of this concept to condensed matter began with the study of Zak of the dynamics of a Bloch electron as its wave vector $k$ changes adiabatically due to an external perturbation until it reaches $k+G$ where $G$ is a reciprocal lattice vector. Although in this case the Hamiltonian which describes the evolution of the periodic part of the Bloch function is noncyclic, the initial and final points are related by a gauge transformation and a Berry phase can be defined for each band, which describes the center of gravity of the density of the Wannier function, or Wyckoff position. Later progress, showed that changes in the macroscopic polarization of a band insulator in an independent particle approximation are proportional to changes in a Berry phase, which I call $\gamma_c$. The formalism was generalized to the many-body case extending previous derivations for quantized charge transport, and was applied to study a ferroelectric transition in a strongly correlated model.

Recently Gagliano and me have introduced the spin Berry phase $\gamma_s$, and have calculated $\gamma_c$ and $\gamma_s$ for the first time in a gapless metallic phase. The model was an extended Hubbard chain with correlated hopping, and due to the presence of inversion symmetry in it, $\gamma_c$ and $\gamma_s$ are quantized and can only have the values 0 and $\pi$. The topological quantum numbers $\gamma_c/\pi$ and $\gamma_s/\pi$ were used as order parameters to construct a phase diagram, separating the three phases of the model: charge-density wave (CDW), spin-density wave (SDW) and the metallic phase. The presence of anomalous flux quantization, and additional arguments, suggest that this phase is superconducting, possibly of triplet character. This work opened the possibility to study phase diagrams in strongly-correlated systems, by looking at topological transitions, which are sharp even in systems of finite size. However, all calculations of $\gamma_c$ and $\gamma_s$ in many-body systems, were so far restricted to an integer number of particles per site. This restriction is too severe, particularly if one is interested in superconductors.

In this Letter, I extend the definition of the Berry phase to the case in which it is necessary to perform more than one cycle in a parameter space, while the Hamiltonian ends at a point related to the starting one by a gauge transformation, in order for the system to return to a state equivalent to the initial ground state. At first sight, this seems to contradict the adiabatic theorem, since there should be a crossing of energy levels before the first cycle ends. However, this crossing is not essential if the matrix element of the Hamiltonian between the states involved vanishes, as it is the case if both states differ in some quantum number. While it seems difficult to imagine a quantum-mechanical system with these properties, the generalization below of the charge Berry phase $\gamma_c$ to systems with fractional number of particles per site is an example. Calculating $\gamma_c$ numerically in a system of 12 sites, I obtain the phase diagram of the extended Hubbard chain for 1/2 particles per site, negative $U$ and any $V$. The results are compared with previous numerical ones, and with analytical ones obtained mapping the model in the limits $|U| \gg t, |V|$ and $|U|, V \gg t$ to Bethe ansatz solvable cases through appropriate canonical transformations. In one dimension (1D), for SU(2) symmetric systems, I show that the spin Berry phase jumps at the boundary between dominating singlet and triplet correlations at large distances, for any filling. For simplicity I restrict the discussion to 1D and one band. Extension to the general case is straightforward.

I consider a system of $L$ sites and number of particles $N$ with $N/L = n/l$, and $n/l$ irreducible. The creation operators satisfy arbitrary boundary conditions for both spins $\hat{c}_{j+L\sigma}^\dagger = e^{i\Phi} \hat{c}_{j\sigma}^\dagger$, and the Hamiltonian $\hat{H}(\Phi_1, \Phi_4)$.
conserves number of particles, $z$ component of the total spin, and is invariant under translations. This invariance allows to define weighted irreducible representations of the translation group characterized by the total wave vector $\mathbf{K} = K + (N_\uparrow \Phi_\uparrow + N_\downarrow \Phi_\downarrow)/L$, where $N_\sigma$ is the number of particles with spin $\sigma$ and $K = \text{integer} \times 2\pi/L$ is one of the allowed wave vectors for periodic boundary conditions (PBC) \cite{PBC}. Using the gauge transformation $c_{j\sigma}^\dagger = e^{-i\Phi_\sigma/L}c_{j\sigma}^\dagger$, the Hamiltonian is converted into one in which the fluxes $\Phi_\sigma$ are distributed equally in each link $H(\Phi_\uparrow, \Phi_\downarrow)$ (the hoppings acquire a phase \cite{phase}), with creation operators satisfying PBC $c_{j\sigma}^\dagger c_{j'+\lambda\lambda\sigma} = c_{j\sigma}^\dagger$. Note that while $\bar{H}(0,0) = \bar{H}(\pm 2\pi, \pm 2\pi), \bar{H}(0,0) = \bar{H}(\pm 2\pi, \pm 2\pi)$ \cite{H00}. To generalize $\gamma_{c}$ ($\gamma_{s}$), the idea is to start from the ground state $|g_{K}(\Phi_\uparrow, \Phi_\downarrow)\rangle$ of $H(\Phi_\uparrow, \Phi_\downarrow)$ for wave vector $K$ and fluxes $\Phi_\sigma$ which minimize the energy, and follow the phase of $|g_{K}\rangle$ as the $\Phi_\sigma$ are shifted adiabatically by the same amount, with the same (opposite) sign, until $|g_{K}\rangle$ reaches a state equivalent to the initial one (the same eigenstate of $\bar{H}$ except for a phase). I discuss first $\gamma_{c}$. It can be defined as $\gamma_{c} = i \sum_{\Phi} \frac{\langle \delta_{\Phi}(g_{K}(\Phi_\uparrow, \Phi_\downarrow)) \rangle}{\langle \delta_{\Phi}(g_{K}(\Phi_\uparrow, \Phi_\downarrow)) \rangle}$, or in the numerically gauge invariant form, discretizing the interval $0 \leq \Phi \leq 2\pi l$ into $M$ points $\Phi_i = 2\pi l$ to $M$ points $\Phi_i = 2\pi l$:  

$$
\gamma_{c} = -\lim_{M \to \infty} \text{Im} \ln \Pi_{i=0}^{M-1} \langle g_{K}(\Phi_{i+1}, \Phi_{i+1})|g_{K}(\Phi_{i+1}, \Phi_{i+1})\rangle \times \langle g_{K}(\Phi_{M-1}, \Phi_{M-1})|e^{-i\sum_{\Phi} c_{i\sigma}^\dagger e_{\sigma}^\dagger}|g_{K}(0,0)\rangle \tag{1}
$$

where the last ket is $|g_{K}(2\pi l, 2\pi l)\rangle$ calculated using the gauge transformation from the eigenstate $|g_{K}(0,0)\rangle$ of $\bar{H}(0,0)$. In practice, $\gamma_{c}$ can be calculated to four digits accuracy using $M \sim 6$ adequately chosen points.

![FIG. 1. Top: Scheme of the evolution of the ground state with flux $\Phi$ for a non-interacting tight-binding model, showing the doubly occupied one-particle states $\vec{k}$ (solid circles) in the one-particle energy dispersion $\epsilon(\vec{k})$. Bottom: Energy as a function of flux of the low-lying energy levels.](image)

In previous cases, $l = 1$ and the integration was restricted to one cycle of $H(0 \leq \Phi \leq 2\pi)$. However, while $K$ is kept fixed, $\bar{K}$ evolves from $K$ to $K + 2\pi n/l$ in this cycle. Since when $l \neq 1$ these $\bar{K}$ are not equivalent, the initial and final states are orthogonal and a Berry phase, even in its more general form \cite{Berry}, cannot be defined for this circuit. In Fig. \ref{fig:1} I illustrate the evolution of the ground state with $\Phi$ for $L = 12$, $n/L = 1/2$ for the case of a non-interacting nearest-neighbor (NN) tight-binding Hamiltonian (Eq. \ref{Ham} for $U = V = 0$). The minimum energy corresponds to $\Phi = 0$. The adiabatic continuation of this state in the representation of $\bar{H}$ as $\Phi$ changes is always the same $|g_{0}(\Phi, \Phi)\rangle = \prod_{\sigma \sigma} c_{-\pi/6\sigma}^\dagger c_{\pi/6\sigma}^\dagger |0\rangle$, where $c_{j\sigma}$ is the Fourier transform of $\gamma_{j\sigma}$. In the representation of $\bar{H}$, each one-particle $\vec{k}$ is shifted by $\Phi/L$ with respect to the corresponding $\vec{k}$. It is easy to see that the energy of $|g_{0}(\Phi, \Phi)\rangle$ is $E_{0}(\Phi) = E(0)\cos(\Phi/L)$, where $E(0)$ is the energy for $\Phi = 0$ \cite{energy}. As $\Phi$ increases from $0$ to $2\pi$, each $\vec{k}$ goes to the next allowed wave vector for PBC, and $|g_{0}\rangle$ evolves to an excited state with $\bar{K} = \pi$. For $\Phi$ near $2\pi$, the ground state is $|g_{\Phi}(\Phi, \Phi)\rangle = \prod_{\sigma} c_{-\pi/3\sigma}^\dagger c_{\pi/3\sigma}^\dagger |0\rangle$ with $\bar{K} = \pi$. The crossing occurs for $\Phi = \pi$ and the ground state energy is of course periodic with period $2\pi$. This crossing does not affect the adiabatic theorem, since the states $|g_{0}\rangle$ and $|g_{\Phi}\rangle$ differ by $K = \pi$. In contrast, $|g_{0}\rangle$ for $\Phi = (2\pi - \theta) + \pi$ represent orthogonal eigenstates of $\bar{H}$ with the same $\bar{K} = 0$ (see Fig. 1) and $\gamma_{c}$ is undefined (one of the factors in Eq. \ref{gamma_c} vanishes). However, since both states have the same quantum numbers, they should hybridize when interactions are present, removing the degeneracy at $\Phi = \pm 2\pi$. In general, for any $L$ and $n/l = 1/2$, the above mentioned states differ in four particles displaced from the neighborhood of the Fermi point $-\pi/4$ to near the other Fermi point $\pi/4$. Umklapp processes of this type are generated in second and higher order perturbation theory in the interaction, and were studied previously \cite{Umklapp}. For other fractional occupancies the situation is similar. The nature of the resulting thermodynamic phase as well as the resulting value of $\gamma_{c}$ depends on the detailed form of the interaction.

I have reexamined the relation between $\gamma_{c}$ and the macroscopic polarization in the present case, following the derivation done previously for $l = 1$ in the many-body case \cite{PBC}. Essential for the extension is to work in a subspace with definite $K$, in such a way that for all $\Phi$ the ground state is separated from the excited states with the same quantum numbers. I obtain that changes in polarization $\Delta P$ are related to the corresponding changes in $\gamma_{c}$ when some parameter of the Hamiltonian varies by:

$$
\Delta P = (e/2\pi l)\Delta \gamma_{c} \pmod{e/l}.
$$

The extra factor $l$ in the denominator is simply due to the $l$ times larger interval of integration in the definition of $\gamma_{c}$. If $H(0,0)$ has inversion symmetry, $H(\Phi_\uparrow, \Phi_\downarrow)$ is transformed to $H(-\Phi_\uparrow, -\Phi_\downarrow)$ under inversion. As a consequence $\gamma_{c} = -\gamma_{c}$ (modulo $2\pi$). This means that in systems with inversion symmetry $\gamma_{c} = 0$ or $\pi$ (modulo...
have large finite-size effects. For example, in the phase energy necessary to add and remove two particles, may the compressibility obtained numerically from the equation and conformal-field theory results [15], which use relation functions vary smoothly at the transition, and to linear combinations of these states (in particular with well defined K). This result suggests that choosing appropriately L one might be able to detect the boundary between S and PS states. Another example in which \( \gamma_c \) is easy to calculate is a CDW for even L in which every second state is singly occupied. Eq. (1) gives \( \gamma_c = \sum_{i=1}^{L/2} \frac{2\pi i}{L} = \pi (L + 2) \equiv 0 \). The same result is obtained if every fourth site is doubly occupied.

The fact that a Berry phase can jump sharply at the boundary between an S phase and a CDW or PS state, can be useful in finite-size diagonalizations, where correlation functions vary smoothly at the transition, and traditional calculations, like those based on bosonization and conformal-field theory results [13], which use the compressibility obtained numerically from the energy necessary to add and remove two particles, may have large finite-size effects. For example, in the phase diagram of the 1D generalized t – J model including a three-site term, a superconducting bubble is predicted inside the PS region, which is an artifact of finite-size effects in the compressibility [4]. Instead, \( \gamma_c \) does not depend on the properties of the system for other densities and has a unique value on the PS state. In other words, although a real phase transition for most systems of interest can only take place in the thermodynamic limit, under certain circumstances, both thermodynamic phases are characterized by different topological quantum numbers, accessible in finite-size systems, and with small size dependence. This was shown in Ref. [14] for a half filled system. Here I calculate \( \gamma_c \) for the following 1D model at quarter filling (\( n/l = 1/2 \)).

\[
H(0,0) = -t \sum_{j \sigma} c_{j+1 \sigma}^\dagger c_{j \sigma} + U \sum_j n_j^\dagger n_j + V \sum_{j \sigma \sigma'} n_{j+1 \sigma} n_{j \sigma'}.
\]

(3)

I restrict most of the study to \( U < 0 \). To distinguish the PS state from the one with dominating singlet superconducting correlations at large distances (S), it turns out that the odd \( N_\sigma \) case mentioned above (leading to \( \gamma_c(PS) = 0 \)) is the convenient choice. Thus, I took \( L = 12 \), \( N_\sigma = N_\uparrow = 3 \), for the numerical calculations. As expected from the above discussion, I obtain in the region \( V > |U| \gg t \), where charge-charge correlations dominate at large distances \( \gamma_c(CDW) = 0 \).

\[
\begin{array}{c}
\gamma_c(PS) = 0
\end{array}
\]

FIG. 2. Charge Berry phase as a function of \( V \) for \( U = -4 \) (dashed line) and \( U = -1 \) (dotted line).

In the S region, \( \gamma_c = 0 \) or \( \pi \) depending on the parameters. Fig. 2 illustrates \( \gamma_c \) as a function of \( V \). There are several jumps in \( \gamma_c \) which do not provide information on phase boundaries. In particular, there is always a jump at \( V = 0 \), and for large \( |U| \) there is another one near \( V = V_c^1 = -t(2)/|U| - 4t^2/|U|^3 \). To illustrate this jump, consider the case \( |U| \gg t, V \). In this limit, it is known that \( H \) reduces to a model of \( N_\sigma \) hard-core bosons, representing doubly occupied sites, which can hop to NN positions with matrix elements \( t'|\pm(\Phi_1 + x\Phi_0)| \), with \( t' = 2t^2/|U| \) (\( t' = -2V_c^2 \) if fourth order corrections are included), and NN repulsion \( V' = 2(2V + t') \). In 1D, each hard-core boson can be mapped into a spinless fermion with an appropriate change in the boundary conditions [17] and this model is equivalent to an XXZ model \( \sum_{<ij>|\alpha} J_{\alpha} S^\alpha_j S^\alpha_i \) with \( N_\sigma \) spins up, and \( J_x = J_y = 2t' \), \( J_z = V' \). Another way to reach the same result is to perform first the unitary transformation \( c_{j \downarrow} = c_{j \uparrow} \), \( c_{j \uparrow} = (-1)^j c_{j \uparrow} \) (which in \( H \) has the effect of changing the sign of \( U \) and \( \Phi_1 \) and transforming the NN repulsion in \( 4V \sum_{<ij>} S^\uparrow_j S^\uparrow_i \), and then eliminate terms linear in \( t \) through a canonical transformation. For \( V' = 0 \) the model can be solved trivially since the interaction vanishes in the spinless-fermion model. Then, one might draw a picture like Fig. 1 to represent \( |\Phi_0(\Phi, \Phi)\rangle \) and again there is a crossing of levels at \( \Phi = \pm 2\pi \) of states with the same \( K = 0 \), but different (singly) occupied (effective) one-particle states \( \tilde{k} \), leading to an undefined \( \gamma_c \). However, in contrast to Fig. 1, states with \( K = \pm \pi/2 \) appear in the low-energy manifold and the ground-state energy as a function of flux \( \Phi \) displays periodicity in \( \pi \) (with minima at \( \Phi = \pi \times \text{integer} \)): the anomalous flux quantization characteristic of the S phase [14,12,18]. A small \( V' \) leads to a well defined \( \gamma_c \) which depends on the...
sign of $V'$. I also find other jumps of $\gamma_c$ for $V = 0$ and at other points inside the S phase, which do not provide information on phase boundaries. The physical meaning of the other jumps inside the S phase is not obvious.

Instead, I find that for $|U| \gg t$, the first and the last transition as a function of $V$ agree very well with the limits of the S phase, obtained in the thermodynamic limit through the exact Bethe-ansatz solution of the equivalent XXZ models: from the solution of the above mentioned XXZ model [13], we know that PS occurs for $J_z < -J_x$ (ferromagnetic Ising-like case), what in terms of the parameters of Eq. (3) means $V < V_{PS} = -2t^2/|U|$. On the other hand, when $V \gg t^2/|U|$, extending previous ideas [17, 3], the entity composed of a doubly occupied site and an empty site right to it can be mapped into a spinless fermion. After an appropriate canonical transformation [13], I find that the resulting spinless fermion model has on-site energy $U - 4t^2/(V - U)$, NN repulsion $V' = 4t^2[1/(V - U) - 1/(3V - U)]$, hopping $t'e^{\pm i(\Phi + \Phi_j)}$, with $t' = 2t^2/(V - U)$, number of particles $N' = N_\sigma = N/2$ and number of sites $L' = L - N/2$. I have calculated the correlation exponent $K_\rho$ of this model in the thermodynamic limit from its compressibility and charge velocity $v_c$ mapped appropriately to the original model [14]. The energy and $v_c$ were obtained solving the corresponding integral equations of the equivalent XXZ model [10]. I obtain that the boundary $K_\rho = 1$ between dominating S or CDW correlations at large distances corresponds to $J_z \cong 0.25J_x$, leading to $V_{CDW} \cong 0.20|U|$. For $5t < |U| < 10t$, I find that for $L = 12$, the first jump in $\gamma_c$ with increasing $V$ is above $V_{PS}$ by $\sim 25\%$ and the last jump is above $V_{CDW}$ by $\sim 15\%$. These numbers are reduced by a factor $\sim 2/3$ if fourth order corrections to $t'$ and $V'$ are included. I believe that the remaining discrepancy is due to finite size effects. For smaller values of $|U|$, the first and last jumps in $\gamma_c$, shown in Fig. 3, agree with previous numerical calculations of $K_\rho$ and compressibility [15, 21]. In correspondence with these calculations, I find an island for high $V$ and small $|U|$ ($V \sim 8t$, $U \sim -2t$, not shown) in which $\gamma_c$ jumps to $\pi$ and $K_\rho > 1$. However, using again an appropriate mapping to two XXZ models, I obtain that this is a finite-size effect and that in the thermodynamic limit the system phase separates into two phases with dominating CDW correlations, in agreement with previous suggestions [18]. One phase is the one just described for $V > V_{CDW}$, and in the other one fermion objects composed of one particle and an empty site next to it move with hopping $t$ and NN attraction $V' = -2t^2/|V|$. Another limit in which the charge dynamics is equivalent to that of interacting spinless fermions is that of $U = +\infty$. Following similar methods as those already used for $V = 0$ [22], the model can be mapped into the spin polarized case $N_\uparrow = L/2$, $N_\downarrow = 0$, with a shift $\Delta \Phi$ in the BC. Calculating $K_\rho$ in the thermodynamic limit, I find that superconducting correlations dominate for $-2t < V < V_{CDW}$, where up to three digits accuracy $V_{CDW} = -\sqrt{2}t$. For $8 \leq L \leq 16$, $\gamma_c$ jumps exactly at this value. Instead, $\gamma_c$ does not detect the transition to the PS state at $V = -2t$ in this case.

In the rest of this Letter, I discuss the spin Berry phase $\gamma_s$. As noted earlier [10, 11], $\gamma_c$ is transformed into $\gamma_s + \pi$ (of a different Hamiltonian in general) and vice versa by the transformation $c_{j\uparrow} = c_{j\uparrow}, \ c_{j\downarrow} = -(1)^j c_{j\downarrow}$. Thus, the definition of $\gamma_s$ can be generalized to $N_\uparrow \neq N_\downarrow$ in the same way as $\gamma_c$, keeping $\Phi_\uparrow = -\Phi_\downarrow$ in the l cycles, and l should be such that $(N_\uparrow - N_\downarrow)/l/L$ is an integer. It is also clear from this transformation and what I obtained for $\gamma_c$ (Eq. (2)) that $\Delta(P_\uparrow - P_\downarrow) = (e/2\pi l)\Delta \gamma_s$ (modulo $e/l$), where $P_\sigma$ is the macroscopic polarization of the particles with spin $\sigma$. If $N_\uparrow = N_\downarrow$, as in most cases of interest, the previous definition of $\gamma_c$ with $l = 1$ [14], is valid for any filling, and for 1D systems with spin SU(2) symmetry, $\gamma_s$ jumps in $\pi$ when a spin gap $\Delta_s$ opens. To show this, I use recent results from continuum limit theory and bosonization [23], which show that the opening of a spin gap is determined by the crossing of the lowest energy states of $H$ with total spin $S = 0$ and $S = 1$ within the $K = 0$ sector, for periodic (antiperiodic) BC if $N_\sigma$ is even (odd). These BC correspond to a particular point $\Phi = \Phi_\uparrow$, with $\Phi_\uparrow = 0$ ($\Phi_\uparrow = \pi$) in the trajectory with $\bar{K} = K = 0$ of $H(\Phi, -\Phi)$ used to define $\gamma_s$. Usually this point corresponds to the maximum of the ground-state energy $E_0(\Phi, -\Phi)$ as a function of $\Phi$, while its minimum lies at $\Phi = \pi$ ($\Phi = 0$) for $N_\sigma$ even (odd), as expected from the non-interacting limit.

From its definition, it is obvious that to calculate $\gamma_s$ any (single valued) $\Phi$-dependent gauge can be chosen. I take the representation in terms of the operators $c_{j\uparrow} = e^{i\Phi_\uparrow/L} c_{j\uparrow}, c_{j\downarrow} = e^{-i\Phi_\downarrow/L} c_{j\downarrow}$, in such a way that in the resulting Hamiltonian $H(\Phi, -\Phi)$, all hoppings are real for
\( \Phi = \Phi_c \) (as in \( \tilde{H}(\Phi_c, -\Phi_c) \)). Sufficiently near to \( \Phi_c \), one can approximate \( \tilde{H}(\Phi, -\Phi) \simeq \tilde{H}(\Phi_c, -\Phi_c) + \frac{\partial \tilde{H}}{\partial \Phi} (\Phi - \Phi_c) \), where the derivative is evaluated at \( \Phi_c \). While at \( \Phi = \Phi_c \), the SU(2) symmetry is conserved, for \( \Phi \neq \Phi_c \) only spin rotations around the quantization axis \( z \) are conserved by \( \tilde{H} \). Specifically, \( \partial \tilde{H}/\partial \Phi \) is equal to the paramagnetic part of the difference between up and down currents, and changes sign under spin rotations in \( \pi \) around the \( x \) or \( y \) axis. I denote these rotations by \( R \) and call \(|s\rangle, E_s \) (\(|t\rangle, E_t \)) the lowest singlet (triplet with spin projection zero) eigenstate of \( \tilde{H}(\Phi_c, -\Phi_c) \) and its energy. It is known that \( R(|s\rangle) = |s\rangle \), and \( R(|t\rangle) = -|t\rangle \). Since \( \partial \tilde{H}/\partial \Phi \) is odd under \( R \), this implies \( \langle s|\partial \tilde{H}/\partial \Phi|s\rangle = \langle t|\partial \tilde{H}/\partial \Phi|t\rangle = 0 \), however, in general \( \langle s|\partial \tilde{H}/\partial \Phi|t\rangle \neq 0 \), where \( A \) can be made real by a suitable change of the phase of one of the states. Near the crossing point between lowest singlet and triplet energies, the ground state \(|g_0(\Phi, -\Phi)\rangle \) results from the diagonalization of the low-energy part \( \tilde{H}_{LE} \) of \( \tilde{H} \) containing the states \(|s\rangle \) and \(|t\rangle \), which according to the above symmetry arguments, has the form:

\[
\tilde{H}_{LE}(\Phi, -\Phi) \simeq \begin{pmatrix}
E_S & A(\Phi - \Phi_c) \\
A(\Phi - \Phi_c) & E_T
\end{pmatrix}.
\]

It is easy to see that this leads to a jump in \( \pi \) in \( \gamma_s \) when \( E_T \) crosses \( E_S \). For example, one can exploit again the gauge invariance to render \( \langle s|\tilde{H}/\partial \Phi|s\rangle \) real and positive for \( \Phi \) near \( \Phi_c \), leading to \(|g_0(\Phi_c + 0^+, -\Phi_c - 0^-)\rangle = -|g_0(\Phi_c - 0^+, -\Phi_c + 0^-)\rangle\) for \( E_S < E_T \) but \(|g_0(\Phi_c + 0^+, -\Phi_c - 0^-)\rangle = -|g_0(\Phi_c - 0^+, -\Phi_c + 0^-)\rangle\) for \( E_S > E_T \) and no other contribution to \( \gamma_s \) in the vicinity of \( \Phi_c \). I obtain numerically in the extended Hubbard model with or without correlated hopping \([10]\) that \( \gamma_s = 0 \) in the spin gapped phase and therefore \( \gamma_s = \pi \) if \( \Delta_s = 0 \). According to continuum limit theory and renormalization group, in 1D, when \( K_p > 1 \), the opening of a spin gap signals the transition from dominating triplet to singlet superconducting correlations at large distance.

In summary, I have shown the ability of two Berry phases, and topological quantum numbers derived from them, to detect phase transitions, particularly in strongly correlated systems with non-integer number of particles per site, for which no previous applications of Berry phases were considered. I hope that this study will stimulate further research and applications of the Berry phases in phase transitions, particularly in dimensions higher than one, where alternative methods which use results of conformal field theory, or exact solutions \([12,13,14,16–20,22]\) are not available.

I am indebted to Gerardo Ortiz for providing me with details of his calculations in Ref. \([3]\) and useful discussions. The numerical diagonalization was done using subroutines developed by Eduardo Gagliano, who unfortunately died on February 12, 1998. I am partially supported by CONICET, Argentina.