Path-integral Monte Carlo for the Gauge-fixed Berry Connection and the Local $Z_2$ Berry Phase

Yuichi Motoyama$^1$ and Synge Todo$^2$

$^1$Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan
$^2$Institute for Solid State Physics, University of Tokyo, 7-1-26-R501 Port Island South, Kobe 650-0047, Japan

E-mail: yomichi@loopert.u-tokyo.ac.jp

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We present a general formula of the gauge-fixed Berry connection which can be evaluated by path-integral Monte Carlo method. We also propose that the gauge-fixed local Berry connection can be another effective tool to estimate precisely the quantum critical point. For a demonstration, we calculate the gauge-fixed Berry connection and the local $Z_2$ Berry phase of the antiferromagnetic Heisenberg model on a staggered bond-alternating ladder, and estimated quantum critical point is consistent with other methods.

KEYWORDS: quantum spin system, quantum phase transition, Berry phase, quantum Monte Carlo, sign problem

1. Introduction

The local $Z_2$ Berry phase, proposed by Hatsugai [1], is a topological order parameter that can characterize a short-range entanglement state such as a spin singlet pair. This is just a Berry phase that the ground state obtains under the local perturbation, for example, only on one bond term. If a model has some symmetry in the space of degree of freedom, this symmetry quantizes the Berry phase. A value of the local Berry phase depends on where the local perturbation works on. For the $S = 1/2$ antiferromagnetic Heisenberg model, for example, the $Z_2$ spin inversion symmetry (time reversal symmetry) quantizes the Berry phase to $0$ or $\pi \text{ mod } 2\pi$. When the local perturbation is bond twist, replacing a bond Hamiltonian on $\langle kl \rangle$ bond $S^+_k S^-_l + S^-_k S^+_l$ by $e^{i\theta} S^+_k S^-_l + e^{-i\theta} S^-_k S^+_l$, the local Berry phase will be $\pi$ or $0$ depending on whether the twisted bond is a valence bond or not in the valence bond solid picture, respectively. Since this quantization is protected by the symmetry, any other perturbation cannot change the Berry phase as long as the energy gap above the ground state remains finite. Therefore, changes of the spatial pattern of $\pi$-valued local quantized Berry phase enable us to catch quantum critical points.

Since the local Berry phase has been calculated only by the exact diagonalization method, the reachable system size is strongly limited especially in higher dimensions and finite size effects remain. Thus, we developed a non-biased large-scale quantum Monte Carlo method for the local quantized Berry phase [2]. We applied the method to an antiferromagnetic Heisenberg model on a staggered bond-alternating ladder [2].

2. Monte Carlo for the Berry connection

In the following, we will derive the evaluation form of the Berry connection by path-integral Monte Carlo method in more general way than one that the authors derived before in the past rapid communication [2]. The ground state of a Hamiltonian $\mathcal{H}(\theta)$ is given by the projection method as
\[ |\Psi(\theta, \sigma)\rangle = \lim_{\beta \to \infty} |\Psi(\theta, \sigma, \beta)\rangle = \lim_{\beta \to \infty} N(\theta, \sigma, \beta)e^{-\beta H(\theta)/2} |\sigma\rangle, \] where \(|\sigma\rangle\) is an arbitrary initial state which is not orthogonal to the ground state, \(\beta > 0\) is a projection parameter, and \(N \in \mathbb{R}\) is a normalization factor. \(\langle \Psi(\theta, \sigma, \beta)|\Psi(\theta, \sigma, \beta)\rangle = 1\). Note that \(|\sigma\rangle\) (more strictly speaking, \(|\sigma(\theta)\rangle\)) fixes the phase of the obtained ground state. By using the path-integral expansion, the inner product between the ground states of two Hamiltonians, \(\mathcal{H}(\theta)\) and \(\mathcal{H}(\phi)\), and the normalization factor can be written in terms of world-line representation as

\[
\tilde{A}(\theta, \phi, \sigma, \beta) \equiv \langle \Psi(\theta, \sigma, \beta)|\Psi(\phi, \sigma, \beta)\rangle = N(\theta, \sigma, \beta)N(\phi, \sigma, \beta) e^{-\beta H(\theta)/2} e^{-\beta H(\phi)/2} |\sigma\rangle \\
= N(\theta, \sigma, \beta)N(\phi, \sigma, \beta) \sum_c W(c, \theta, \phi, \sigma, \beta) \\
= N_\theta N_\phi \sum_c W(c, \theta, \phi) \\
\equiv N_\theta N_\phi \sum_c W(c, \theta, \phi)
\]

with \(N_\theta^{-2} = \sum_c W(c, \theta, \theta)\), where \(c\) is the index of world-line configurations and \(W\) is the weight function. From this point, we will omit \(\sigma\) and \(\beta\) like the last line of eq. (1) for simplicity.

The derivative of the inner product \(\tilde{A}\) gives us the gauge fixed Berry connection,

\[
A(\theta) \equiv \left(\frac{\partial |\Psi(\theta)\rangle}{\partial \theta} \right|_{\theta=\phi} |\Psi(\theta)\rangle = \left. \frac{\partial \tilde{A}(\theta, \phi)}{\partial \phi} \right|_{\phi=\theta} \\
= N_\theta N_\phi \sum_c \frac{\partial W(c, \theta, \phi)}{\partial \phi} + N_\theta \frac{\partial N_\phi}{\partial \phi} \sum_c W(c, \theta, \phi) \bigg|_{\phi=\theta} \\
= N_\theta^2 \sum_c \frac{\partial W(c, \theta, \phi)}{\partial \phi} \bigg|_{\phi=\theta} + N_\theta \frac{\partial N_\phi}{\partial \phi} \sum_c W(c, \theta, \theta). 
\]

The complex conjugate of the Berry connection can be obtained in the same way,

\[
A^*(\theta) \equiv \left(\frac{\partial |\Psi(\theta)\rangle}{\partial \theta} \right|_{\theta=\phi} |\Psi(\theta)\rangle^\ast = \left. \frac{\partial \tilde{A}(\theta, \phi)}{\partial \theta} \right|_{\theta=\phi} = N_\theta^2 \sum_c \frac{\partial W(c, \theta, \phi)}{\partial \theta} \bigg|_{\theta=\phi} + N_\theta \frac{\partial N_\phi}{\partial \theta} \sum_c W(c, \theta, \theta). 
\]

Since the Berry connection is pure imaginary, the difference between it and its complex conjugate is just twice as much as itself, so the Berry connection is given by

\[
A(\theta) = \frac{A(\theta) - A^*(\theta)}{2} = \frac{1}{2} \left( \frac{\partial}{\partial \theta} - \frac{\partial}{\partial \phi} \right) \tilde{A}(\theta, \phi) \bigg|_{\phi=\theta} \\
= \frac{N_\theta^2}{2} \sum_c \left( \frac{\partial}{\partial \theta} - \frac{\partial}{\partial \phi} \right) W(c, \theta, \phi) \bigg|_{\phi=\theta} \\
= \frac{1}{2} \sum_c \left( \frac{\partial}{\partial \theta} - \frac{\partial}{\partial \phi} \right) W(c, \theta, \theta). 
\]

Unfortunately, this general form cannot be evaluated directly by Monte Carlo method.

Now, we will consider a special case; an antiferromagnetic Heisenberg model with local twist. In this model, the Hamiltonian of which is \(\mathcal{H}(\theta) = J \sum_{i,j \in k \cdot \theta} S_i^+ S_j^- + J S_I^+ S_I^- + J(\epsilon_{\sigma} S^+_I \hat{S}^-_I + e^{-\beta} S^-_I \hat{S}^+_I)\),

the weight function can be decomposed to a parameterized phase factor and a weight function without parameters, \(W(c, \theta, \phi) = \exp(i \epsilon n_{\epsilon}^{\hat{U}} + i \epsilon n_{\epsilon}^{\hat{W}}) W_0(c)\), where \(n_{\epsilon}^{\hat{U}}\) is the difference between the number of \(S^+_I \hat{S}^-_I\) and that of \(S^-_I \hat{S}^+_I\) at \(\tau < \beta/2\) and \(n_{\epsilon}^{\hat{W}}\) is one at \(\tau > \beta/2\). \(W_0(c)\) is an abbreviation of \(W(c, 0, 0)\), which is the same as an ordinary Heisenberg model except for the boundary condition along to the
imaginary-time direction (fixed in the present method and periodic in the ordinary one.) Finally, we
succeed to derive a Monte Carlo evaluation formula for the Berry connection,

\[ A(\theta) = \frac{\sum_c i n_c e^{i\theta n_c^*} W(c, 0, 0)}{2 \sum_c e^{i\theta n_c} W(c, 0, 0)} = \frac{i \sum_c n_c e^{i\theta n_c^*} W_0(c)}{2 \sum_c W_0(c)} \]

\[ = \frac{i \langle n^* e^{i\theta n^*} \rangle}{2 \langle e^{i\theta n^*} \rangle}, \tag{5} \]

where \( n^\pm = n^U \pm n^L \) and \( \langle O \rangle \) is the expectation value of \( O \) over the Monte Carlo simulation with \( \theta = 0 \).

This Monte Carlo expectation form, of course, suffers from a “complex weight problem.” This
problem arises as the denominator of this will have an exponentially small expectation value and
an constant-order variance when the projection parameter \( \beta \) becomes larger. Fortunately, at some
parameter \( (\theta/\pi = p/q \text{ where } p \text{ and } q \text{ are mutually prime and } q \text{ is even}) \) the meron cluster algorithm
can be applied to this sign problem, and we can calculate the Berry phase from those discrete data by
numerical integration [2].

3. Demonstration

To demonstrate the present method, we calculated the antiferromagnetic Heisenberg model on a
staggered bond-alternating ladder. The Hamiltonian is

\[ \mathcal{H} = \sum_{j=1}^{L} \left[ J \left(1 + (-1)^j \delta \right) S_{1,j} \cdot S_{1,j+1} + J \left(1 - (-1)^j \delta \right) S_{2,j} \cdot S_{2,j+1} + J' S_{1,j} \cdot S_{2,j} \right], \tag{6} \]

where \( L \) is the ladder length (and so the number of sites is \( N = 2L \)) and \( S_{i,j} \) stands for the \( S = 1/2 \)
spin operator on the \( j \)-th site of the \( i \)-th leg. The boundary condition along the ladder is periodic,
that is, \( S_{i,L+1} = S_{i,1} \) (\( i = 1, 2 \)). Depending on the strength of rung coupling the spatial pattern of the
valence bond changes. When rung coupling is weak, \( J' < J'(\delta) \), valence bonds are on all strong leg
bonds \( (J(1 + \delta) \text{ bonds). Otherwise, } J' > J'(\delta) \), they are on rung bonds. The threshold \( J'(\delta) \) is the
quantum critical point [3]. In the present study, we fix \( J = 1 \) and \( \delta = 0.5 \), for which the quantum
critical point has been estimated as \( J' \sim 1.2 \) [4].

Figure 1 shows the Berry phase calculation for system sizes \( L = 8, 16, 32 \) and projection parameter
\( \beta = 2L \). When the rung coupling becomes larger, the local Berry phase on the strong leg bonds
\( \gamma^\text{leg} \) and the rung bonds \( \gamma^\text{rung} \) varies from \( \pi \) to 0 and from 0 to \( \pi \), respectively. Since the projection
parameter is not so large close to the critical point that projected states do not reach the ground states,
these curves are not step functions. In this case, however, since the energy gap remains finite except
at the critical point, the curves converge to step functions as \( L \) and \( \beta \) become larger.

To estimate the critical point, we observed the size dependency of three points: \( J_c^\text{leg}(L) \) and
\( J_c^\text{rung}(L) \) are the points where \( \gamma^\text{leg} = \pi/2 \) and \( \gamma^\text{rung} = \pi/2 \), respectively, and \( J_c^\text{cross}(L) \) is the one where
\( \gamma^\text{leg} = \gamma^\text{rung} \). The critical point in the thermodynamics limit, \( J_c^* \), is estimated by size extrapolation of
\( J_c(L) \) for lattice sizes up to \( L = 32 \): \( J_c^\text{leg} = 1.2281(18) \), \( J_c^\text{rung} = 1.2282(18) \), and \( J_c^\text{cross} = 1.2266(6) \)
(Fig. 2). These results are consistent within statistical errors with the independent finite-size scaling
(FSS) analysis for the staggered susceptibility, \( J_c^* / J = 1.2268(2) \).

Figure 3 shows the leg twist gauge-fixed Berry connection with twist angle \( \theta = 0 \). It is clear that
the three curves, \( L = 128, 192, 256 \), cross at one point, \( J' = 1.227(1) \). Under the gauge transformation,
Fig. 1. The local Berry phase of the staggered ladder with system size $L = 8$ (squares), 16 (circles), and 32 (triangles) on the leg bonds (solid red symbols) and the rung bonds (open blue symbols). The projection parameter $\beta$ is $2L$ [2].

Fig. 2. The estimation of the critical point of staggered ladders obtained by the local $Z_2$ Berry phase on the leg bond (circles), rung bond (triangles), and their crossing point (squares). The horizontal line, $J'/J = 1.2268$, is the FSS result of staggered susceptibility [2].

Fig. 3. The leg twist gauge-fixed Berry connection of the staggered ladder with system sizes $L = 128, 192, 256$ and projection parameter $\beta = 2L$. The crossing point is $J' = 1.227(1)$.

$|\psi(\theta)\rangle \rightarrow e^{i\chi(\theta)}|\psi(\theta)\rangle$, the Berry connection varies as $A(\theta) \rightarrow A(\theta) + i\partial_\theta \chi(\theta)$, where $\chi$ is some arbitrary periodic real function such as $\chi(\theta) = \chi(\theta + 2\pi)$. This means that the gauge transformation shifts the $J'$-$A$ curve only vertically by a constant and does not change the crossing point. Thus, the permitted finite size scaling is only $J'$ rescaling, such as $A(J', N) = f((J' - J'_c)N^{1/\nu})$, with some universal function $f$. Figure 4 shows the result of the finite size scaling result of the gauge-fixed Berry connection at $\theta = 0$. The system sizes are $L = 128, 192, 256$ and the projection parameter is $\beta = 2L$. The scaling parameters are $J'_c = 1.2268(1)$ and $\nu = 0.738(8)$ for the leg twist and $J'_c = 1.2265(1)$ and $\nu = 0.747(10)$ for the rung twist. These estimates agree with the result of the finite size analysis of staggered susceptibility obtained by loop algorithm.
4. Conclusion

We presented the Monte Carlo form of the gauge-fixed Berry connection and used it to calculate the local $Z_2$ Berry phase. We also proposed that the gauge-fixed Berry connection can be used as an effective tool to catch the quantum phase transition. For the demonstration, we applied these to the antiferromagnetic Heisenberg model on a staggered bond-alternating ladder. The estimated critical point is consistent with the finite size analysis of staggered susceptibility.

We used ALPS libraries [5,6] to develop the simulation code and ALPS application (ALPS/looper [7, 8]) to calculate the staggered susceptibility to check our result. We also used BSA [9,10] for Bayesian finite size analysis. We acknowledge support by KAKENHI (No. 23540438), JSPS, Grand Challenges in Next-Generation Integrated Nanoscience, Next-Generation Supercomputer Project, the HPCI Strategic Programs for Innovative Research (SPIRE), the Global COE program “the Physical Sciences Frontier,” MEXT, Japan, and the Computational Materials Science Initiative (CMSI).

References

[1] Y. Hatsugai: J. Phys. Soc. Jpn. 73 (2004) 2604.
[2] Y. Motoyama and S. Todo: Phys. Rev. E 87 (2013) 021301(R).
[3] M. A. Martín-Delgado, R. Shankar, and G. Sierra: Phys. Rev. Lett. 77 (1996) 3443.
[4] K. Okamoto: Phys. Rev. B 67 (2003) 212408.
[5] B. Bauer and et al.: J. Stat Mech. (2011) P05001.
[6] http://alps.comp-phys.org/.
[7] S. Todo and K. Kato: Phys. Rev. Lett. 87 (2001) 047203.
[8] http://wistaria.comp-phys.org/alps-looper/.
[9] K. Harada: Phys. Rev. E 84 (2011) 056704.
[10] http://kenjiharada.github.io/BSA/.