Mitigating sign problem by automatic differentiation

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As an intrinsically-unbiased method, quantum Monte Carlo (QMC) is of unique importance in simulating interacting quantum systems. Unfortunately, QMC often suffers from the notorious sign problem. Although generically curing sign problem is shown to be hard (NP-hard), sign problem of a given quantum model may be mitigated (sometimes even cured) by finding better choices of simulation scheme. A universal framework in identifying optimal QMC schemes has been desired. Here, we propose a general framework using automatic differentiation (AD) to automatically search for the best continuously-parameterized QMC scheme, which we call “automatic differentiable sign mitigation” (ADSM). We further apply the ADSM framework to the honeycomb lattice Hubbard model with Rashba spin-orbit coupling and demonstrate ADSM’s effectiveness in mitigating its sign problem. For the model under study, ADSM leads a significant power-law acceleration in computation time (the computation time is reduced from $M$ to the order of $M^\nu$ with $\nu \approx 2/3$).

Introduction: Numerical study of quantum systems is of vital importance, especially in the context of strongly correlated systems which are in general analytically intractable. Due to their exponentially growing Hilbert space, numeric methods such as exact diagonalization usually fail when their system size is moderately large. Nonetheless, quantum Monte Carlo (QMC) can putatively overcome such “exponential wall” by accessing a fraction of Hilbert space stochastically. QMC is intrinsically unbiased, making it one of the most powerful and successful methods to simulate many-body systems. Unfortunately, QMC is often plagued by the notorious sign problem when dealing with fermion systems or frustrated spin models [1–3]. When sign problem occurs, the simulation uncertainty increases exponentially with the system size and inverse temperature, rendering it infeasible in simulating systems at low-temperature or with large size [4–10]. It has been desired for many decades to cure the sign problem of interacting models such as the Hubbard model at generic filling so that physical properties such as high-temperature superconductivity may be studied by the intrinsically-unbiased method of QMC.

Tremendous progress has been made to cure sign problem by identifying sign-free QMC schemes for models with certain symmetries [11–15] (see, e.g., Ref. [16] for a recent review). Fruitful physics has been revealed in studying these fermion models by sign-problem-free QMC (see, e.g., Refs. [17–50]). Nonetheless, generically solving sign problem is almost as it has been proved that the sign problem complexity is NP-hard [51]. Moreover, it was shown recently that interacting models whose ground states feature certain properties such as gravitational anomaly may have intrinsic sign problem; namely sign problem of these models cannot be cured [52–55]. Fortunately, for a given model it is possible to mitigate its sign problem even when it cannot be completely cured. Effort along this direction has been made recently; sign problem mitigation was studied using basis transformation [56–62], Lefschetz thimbles [63–65] and machine learning techniques [66–68]. However, a universal framework of mitigating sign problem for interacting fermion systems is still lacking.

Here we fill in this gap by constructing a general framework of sign mitigation in determinant quantum Monte Carlo (DQMC). DQMC was introduced by Blankenbecler, Scalapino, and Sugar (BSS) [69] and has been extensively used in simulating interacting lattice fermion models. It has been known that sign problem in DQMC crucially depends on the scheme of performing Hubbard-Stranovichi (HS) transformation. Different forms of HS transformations were proposed in the early stage of developing DQMC and simulating models like the Hubbard model [5, 70–73]. Nonetheless, previous HS transformations employed in practical simulations are quite limited in forms and are constrained to no spatial dependence. By constructing sufficiently general HS transformations and finding the optimal one, sign problem of a given model may be improved or mitigated.

We propose a general framework to realize sign mitigation by parameterizing HS transforms continuously and optimizing (mitigating) the sign using automatic differentiation (AD) [74–76]. We call it “automatic differentiable sign mitigation” (ADSM). (AD is a powerful method for optimization that is widely encountered in machine learning and features various applications in computational physics [77–86].) ADSM is a general framework in mitigating sign problem, applicable to essentially all quantum models. We demonstrate the ADSM framework by applying it to the honeycomb Hubbard model with Rashba spin-orbit couplings to mitigate its sign problem. For the Rashba-Hubbard models we study, the mitigated sign leads to a significant power-law acceleration (the computation time is reduced from $M$ to approximately the order of $M^\nu$ with $\nu \approx 2/3$).

DQMC and sign problem: DQMC is widely used in simulating interacting fermion models. To study equilib-
rium properties of an interacting fermion model described by Hamiltonian $\hat{H}$, one normally computes the expectation value of some observable $\hat{O}$: $\langle \hat{O} \rangle = \frac{\text{Tr}(\hat{O} e^{-\beta \hat{H}})}{\text{Tr}(e^{-\beta \hat{H}})}$, where $\beta = 1/T$ is the inverse temperature. Using the Suzuki-Trotter decomposition [87, 88] along the imaginary time direction, we obtain the density matrix $e^{-\beta \hat{H}} = \prod_{s=0}^{L-1} e^{-\Delta \tau \hat{H}} \simeq \prod_{s=0}^{L-1} e^{-\Delta \tau \hat{H}_0} e^{-\Delta \tau \hat{H}_1}$, where $\beta = L \Delta \tau$ and $\hat{H} = \hat{H}_0 + \hat{H}_1$ with $\hat{H}_0$ the quadratic term and $\hat{H}_1$ the quartic or interacting term. To deal with the quartic term $\hat{H}_1$, one can convert it into quadratic forms by performing HS transformations; the price to pay is the introduction of auxiliary fields. A general form of HS transformation is given by

$$e^{-\Delta \tau \hat{H}_1} = \sum_s \eta(s) e^{V(s)},$$  

(1)

where $s$ represents auxiliary fields, $V(s) = c^\dagger V(s)c$ are quadratic fermion operators with the matrix $V(s)$ and fermion creation operators $c^\dagger$ (indices in $c^\dagger$ are implicitly included), and $\eta(s)$ is a prefactor. Here we assume $s$ take some discrete values, though continuously-valued auxiliary fields [89] can also be treated in ADSM. With HS transformation at every time slice $l$, we obtain the HS decoupled form of the density matrix: $e^{-\beta \hat{H}} = \sum_s \prod_{l=0}^{L-1} \eta(s_l) e^{-\Delta \tau \hat{H}_0} e^{-\Delta \tau V(s_l)} = \sum_s \hat{\rho}_s$, where $s$ represent auxiliary fields configuration $\{s_l\}$ and the summation is over all possible auxiliary field configurations $s$.

Then, the expectation value of $\hat{O}$ is given by $\langle \hat{O} \rangle = \frac{\text{Tr}(\hat{O} \hat{\rho}(s))}{\text{Tr}(\hat{\rho}(s))} = \text{Tr}(\hat{\rho}(s)) = \sum_s w(s) O(s)$, where $O(s)$ is the expectation of observable $\hat{O}$ in the auxiliary field configuration $s$ and $w(s) = \text{Tr}(\hat{\rho}(s)) = \eta(s) \det(1 + \prod_{l=0}^{L-1} e^{K e^{V(s_l)}})$ is the Boltzmann weight of auxiliary field configuration $s$ with $K$ the matrix obtained from $-\Delta \tau \hat{H}_0 = c^\dagger Kc$ and $\eta(s) = \prod_{l=0}^{L-1} \eta(s_l)$. To obtain $\langle \hat{O} \rangle$ by QMC, one computes the expectation of $O(s)$ with $s$ sampled from an unnormalized distribution $w(s)$, namely $\langle \hat{O} \rangle = \langle O(s) \rangle_{s \sim w(s)}$. However, there is no guarantee that $w(s)$ is always positive. When $w(s)$ can take both positive and negative (sometimes complex) value, it is so-called sign problem.

When sign problem appears, the absolute value of $w(s)$ can be used to sample the configurations by absorbing the sign or phase factor $e^{i \phi(w(s))} = w(s)/|w(s)|$ into observable: $\langle O(s) \rangle_{s \sim w(s)} = \langle e^{i \phi(w(s))} O(s) \rangle_{s \sim |w(s)|} = \langle e^{i \phi(w(s))} \rangle_{s \sim |w(s)|}$, where the denominator and numerator can be calculated stochastically using Markov chain Monte Carlo with the auxiliary fields sampled from the distribution $|w(s)|$. The denominator is so-called average sign $S$ in QMC: $S \equiv \langle e^{i \phi(s)} \rangle_{s \sim |w(s)|} = \sum_s w(s)/\sum_s |w(s)|$. As the partition function $Z = \text{Tr}(e^{-\beta \hat{H}}) = \sum_s w(s)$ is always positive, the average sign $S$ must be positive and it can be easily proved that $0 < S \leq 1$. It was observed [4] that the average sign decays exponentially with system size $N$ and inverse-temperature $\beta$ as $S \sim e^{-\kappa N \beta}$ for sufficiently large $N$ and $\beta$, where $\kappa$ is a constant. For sign-problematic (sign-free) QMC, $\kappa > 0$ ($\kappa = 0$). When sign problem occurs, to obtain the value of $\langle \hat{O} \rangle$ within a given accuracy the needed QMC simulation time $M$ increases exponentially with size and inverse temperature:

$$M \sim \frac{1}{S^2} \sim e^{2\kappa N \beta}.$$  

(2)

This greatly hinders feasibility of applying QMC to study interacting systems with large size or low temperature.

The ADSM framework: The average sign $S$ or the prefactor $\kappa$ discussed above is not an intrinsic property of a quantum model itself; instead it crucially depends on how the HS transformation is performed in the DQMC scheme. For a given model, a smaller $\kappa$ implies less severe sign problem. In other words, mitigating sign problem is equivalent to reducing $\kappa$ by identifying an optimal HS transformation. Suppose we have a set of possible HS transformations that can be parameterized using some continuous parameters $\xi$, the form of HS transformation in Eq. (1) now becomes

$$e^{-\Delta \tau \hat{H}_1} = \sum_s \eta(\xi,s) e^{V(\xi,s)} = \sum_s \eta(\xi,s) e^{c^\dagger V(\xi,s)c}.$$  

(3)

Consequently, $w(\xi,s) = \eta(\xi,s) \det(1 + \prod_{l=0}^{L-1} e^{K e^{V(\xi,s)}})$, $S(\xi)$, and $\kappa(\xi)$ can all depend on the HS parameters $\xi$. Sign mitigation becomes an optimization problem in the parameter space of $\xi$.

Here we choose $\ln S$ instead of $S$ itself as our objective function. We would like to maximize $\ln S$ (equivalently maximizing $S$ itself). We do not use $S$ directly because it may lead to the vanishing gradients due to the exponential smallness of $S$. Using the fact that the partition function $Z$ of a model is independent with $\xi$, we obtain the differentiation of $\ln S$ as (see the SM for details)

$$d \ln S = -\text{Re} \left( \frac{d w(\xi,s)}{w(\xi,s)} \right)_{s \sim |w(\xi,s)|}.$$  

(4)

Note that sign averaging is not involved in Eq. (4), which means computing the gradients itself is actually sign-problem-free. It is interesting that gradients of $\ln S$ could be efficiently and reliably calculated even though it is difficult to accurately compute $S$ itself. In other words, our sign mitigation framework is itself sign-problem-free; thus the mitigation framework can be directly applied on large size systems of interest.

It seems that the differentiation $\frac{d w(\xi,s)}{w(\xi,s)}$ can be directly achieved using reverse-mode AD since the forward output $w(\xi,s)$ can be calculated as a determinant. But it is actually trickier than that due to numerical instability of matrix production within determinants. Since the forward evaluation of $w(\xi,s)$ is plagued by lots of numerical stabilization procedures such as pivoted QR, it is hard to directly obtain the gradient via simple backpropagations.
To address this problem, we further write the gradient as:
\[
\frac{d\ln \mathcal{L}(\xi, \mathbf{s})}{\partial \mathbf{s}} = \frac{d\ln \mathcal{L}(\xi, \mathbf{s})}{\partial \mathbf{s}} + d \ln \det \left[ \mathbb{I} + B(\xi, \mathbf{s}) \right]
\]
\[
= \frac{d\ln \mathcal{L}(\xi, \mathbf{s})}{\partial \mathbf{s}} + \sum_{l=0}^{L-1} \text{Tr} \left[ \mathcal{G}_l(\xi, \mathbf{s}) B_l(\xi, \mathbf{s})^{-1} dB_l(\xi, \mathbf{s}) \right],
\]
where \( B(\xi, \mathbf{s}) = \prod_{l=0}^{L-1} B_l(\xi, s_l) \), \( B_l(\xi, s_l) = e^{K e \mathcal{V}(\xi_{-l})} \), and \( \mathcal{G}_l = \left[ \mathbb{I} + (B_{l-1} \cdots B_0)^{-1}(B_{l-1} \cdots B_0)^{-1} \right]^{-1} \). The form of \( \mathcal{G}_l \) is also encountered in usual DQMC when calculating equal-time Green’s functions. Pivoted QR decomposition [90–93] are recursively used to stabilize the matrix productions. The decompositions \( B_{l-1} \cdots B_0 = U_R D_R V_R \) and \( B_{l-1} \cdots B_l = V_l D_l U_l \) are utilized as in standard DQMC algorithm, where \( U, V \) are supposed to be well-conditioned and \( D \) is a diagonal matrix. \( \mathcal{G}_l \) can be calculated in numerically stable fashion using these by-products (see the SM for details). Therefore, only very few computational resources in addition to standard DQMC algorithm are required in our ADSM framework.

Now we have all the ingredients to calculate the gradients. Fig. 1 represents a schematic diagram of the whole ADSM framework. It is worth noting that we also need score function/REINFORCE method for AD since the forward evaluation is involved with Monte Carlo sampling [86, 94, 95]. Stochastic gradients descent (SGD) is suitable in our case to optimize the target function \( \mathcal{L} \) since the gradients are calculated in a stochastic way: \( \xi \rightarrow \xi + \delta \nabla \mathcal{L} \ln \mathcal{L} \), where \( \delta \) is the learning rate.

The Rashba-Hubbard model: We further apply our general ADSM framework to the honeycomb Hubbard model with Rashba spin-orbit couplings [96]. The Hamiltonian of the Rashba-Hubbard model is given by
\[
\mathcal{H} = -t \sum_{\langle ij \rangle} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta} + \lambda_R \sum_{\langle ij \rangle} \hat{\xi} \cdot (\sigma_{\alpha\beta} \times \mathbf{d}_{ij}) \hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta} + U \sum_i (n_i^\uparrow - \frac{1}{2})(n_i^\downarrow - \frac{1}{2}),
\]
where \( \hat{c}_{i\alpha}^\dagger \) creates an electron on site \( i \) of the honeycomb lattice with spin polarization \( \alpha = \uparrow, \downarrow \), \( n_{i\sigma} = \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} \), \( (ij) \) labels the nearest neighbor sites \( i \) and \( j \), \( \sigma \) represent Pauli matrices, and \( \mathbf{d}_{ij} \) is the vector pointing from spatial sites \( i \) to \( j \). Hereafter we set the NN hopping \( t = 1 \) as energy unit unless stated otherwise. \( \lambda_R \) is the Rashba spin-orbit coupling and \( U \) is the Hubbard interaction. This model can be relevant to certain realistic materials as the Rashba spin-orbit coupling has been observed in graphene interface [97, 98]. The model is invariant under the particle-hole transformation \( c_{i\sigma} \rightarrow (-1)^{\mathbf{r} \cdot \mathbf{L}} c_{i\sigma}^\dagger \); thus the system is at half filling. For \( \lambda_R = 0 \), the model respects SO(3) spin-rotational symmetry and is known to be sign-problem free. For \( \lambda_R \neq 0 \), however, this model is known to be sign problematic. A natural question to ask is what HS transformation can give rise to the most mitigated sign problem when \( \lambda_R \neq 0 \).

We consider HS transformations with the auxiliary fields on each site \( i \) coupled to spin operators which are parameterized by a unit vector \( \mathbf{n}_i \):
\[
e^{-\Delta \tau U(n_i^\uparrow - \frac{1}{2})(n_i^\downarrow - \frac{1}{2})} = \frac{1}{2} e^{-U \Delta \tau / 4} \sum_{n_i = -1}^1 e^{\lambda_s c_{i\sigma}^\dagger \mathbf{n}_i \cdot \mathbf{c}_i \cdot n_{i\sigma}},
\]
where two continuous parameters \( \theta_i \) and \( \phi_i \) are introduced on each site \( i \) to characterize the unit vector \( \mathbf{n}_i = (\sin \theta_i, \sin \phi_i, \sin \theta_i \cos \phi_i, \sin \theta_i \cos \phi_i) \). The parameters on each site feature the equivalence \( \mathbf{n}_i \equiv -\mathbf{n}_i \) by symmetry. Note that, in trying to optimizing for the best HS transformations, the ADSM framework will allow spatially non-uniform \( \mathbf{n}_i \).
First, we apply the ADSM method to a relatively small system size with $3 \times 3 \times 2$ sites and periodic boundary condition. We choose $U = 6$ and $\beta = 5$ in the calculations. In generally used scheme of HS transformations, $\mathbf{n}_i = \hat{z}$ is spatially uniform. Using ADSM, the optimized signs for $\lambda_R = 0.5$ and $\lambda_R = 1.0$ are presented in Fig. 2(a) and Fig. 2(c), respectively. It is clear that for both cases the sign is significantly improved using our framework. The optimized HS transformation, unlike the previously used uniform $\mathbf{n}_i = \hat{z}$ decoupling scheme, is not spatially uniform, as shown in Fig. 2(b) and Fig. 2(d). Moreover, the optimal pattern of $\mathbf{n}_i$ can be different for different model parameters, which implies that the optimal pattern may be related to the properties of its underlying phases.

Next, we will check whether the optimized HS transformation obtained for the $3 \times 3 \times 2$ lattice is similar to the one for larger system size. If the optimized HS transformation does not change dramatically with system size, the optimized pattern obtained for relatively small system size can be directly used to perform QMC simulations on larger system size. For $\lambda_R = 1.0$, the HS transformations can be constrained to $\theta_i = \theta, \phi_i = \phi$ for $i$ on A sublattice and $\theta_i = -\theta, \phi_i = \phi$ for $i$ on B sublattice, where $\theta$ and $\phi$ can vary to obtain the optimized sign. We then check if the optimized values of $\theta$ and $\phi$ are similar for different system sizes. As shown in Fig. 3(a) and Fig. 3(b), respectively, $\theta$ and $\phi$ are converged to almost the same value for different system sizes.

As shown in Fig. 4(a), the larger system size is, the greater the sign problem improves. This indicates that the optimized HS transformation can reduce the prefactor $\kappa$ compared to the uniform $\mathbf{n}_i = \hat{z}$ scheme. Sign mitigation can be quantitatively characterized by how much the exponential prefactor $\kappa$ is reduced from optimizing HS transformations. We use $\kappa^*$ to denote its value in the optimized HS transformation scheme and $\kappa_0$ the value in spatially uniform HS scheme without optimization. As the MC computation time $M$ scales as $M \sim \frac{1}{\kappa^*} \sim e^{2\kappa N \beta}$, it implies that the computation can be power-law accelerated from $M$ to the order of $M^\nu$, where $\nu = \kappa^*/\kappa_0$.

For $\lambda_R = 1.0$ and $U = 6.0$, we compare the scaling of the average sign $S$ versus $\beta$ and $N$, between the previously used HS scheme and the ADSM optimized one, as shown in Fig. 4. We obtain $\nu = \kappa^*/\kappa_0 \approx 0.64 \sim 0.71$ for $\lambda_R = 0.5 \sim 1.0$. The power-law acceleration with $\nu \approx 2/3$ can lead to tremendous acceleration when the system is large or temperature is low. For instance, when $U = 6.0$ and $\lambda_R = 1.0$, for the relatively small lattice with $N = 5 \times 5 \times 2 = 50$ sites and moderately high temperature $\beta = 5$ the acceleration is already huge; it is about $(S^*/S_0)^2 \sim 3 \times 10^5$ times faster, where $S_0$ represents the average sign obtained in the usual HS scheme and $S^*$ in the optimized one.

### Discussions and concluding remarks:

The general framework of mitigating sign problem of DQMC proposed in the present work can be used in principle in any interacting quantum systems as long as its HS transformation can be continuously parameterized. For instance, by enlarging auxiliary field space or allowing hybrid decoupling schemes, further sign optimization may be obtained (see the SM for details). Moreover, the general idea of AD can be further applied to other types of QMC methods including world-line MC and hybrid MC whenever continuous parametrization can be implemented.

As ADSM provides a general framework to mitigate sign problem of interacting models and it worked well for the Rashba-Hubbard model, it is desired to apply it to other strongly correlated models whose solutions remain elusive so far. One future direction is to apply ADSM to mitigate sign problem of the doped Hubbard model on square lattice so that its low temperature properties including possible pseudogap phenomena and high-temperature superconductivity [99] may be reliably probed using ADSM-optimized QMC scheme.
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A. Continuously-parameterized HS transformations

Continuous parametrization of HS transformations is essential to the ADSM framework. It is important to find a sufficiently general HS transformation which is able to give rise to reasonably good sign. We present a few parameterization approach below where we use the Hubbard interaction as an example for most cases.

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SUPPLEMENTAL MATERIALS

A. Continuously-parameterized HS transformations

Continuous parametrization of HS transformations is essential to the ADSM framework. It is important to find a sufficiently general HS transformation which is able to give rise to reasonably good sign. We present a few parameterization approach below where we use the Hubbard interaction as an example for most cases.

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1. Gauged HS transformation

Gauged HS transformation was introduced in Ref. [73]. It was noticed that there exists some freedom in the conventional discrete HS transformations of the Hubbard interactions. For the repulsive case \((U > 0)\):

\[
e^{-U \Delta \tau(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})} = \frac{b}{2} e^{-U \Delta \tau / 4} \sum_{s_{\uparrow}, s_{\downarrow} \in \{-1, 1\}} \exp(-\xi s_{\uparrow} s_{\downarrow} + \xi s_{\uparrow} (2n_{\uparrow} - 1) + s_{\downarrow} (2n_{\downarrow} - 1)),
\]

where \(c^\dagger = (c_{\uparrow}^\dagger, c_{\downarrow}^\dagger)\) is a normal spinor, \(\cosh \lambda = \exp(U \Delta \tau / 2)\), and \(\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)\). Here \(\mathbf{n}\) or \((\theta, \phi)\) are the continuous parameters that characterize the HS transformation. For the attractive case \((U < 0)\):

\[
e^{-U \Delta \tau(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})} = \frac{b}{2} e^{-|U| \Delta \tau / 4} \sum_{s_{\uparrow}, s_{\downarrow} \in \{-1, 1\}} e^{\lambda s_{\uparrow} \mathbf{n} \cdot \mathbf{\psi}},
\]

where \(\mathbf{\psi} = (c_{\uparrow}^\dagger, c_{\downarrow}^\dagger)\) is a Nambu spinor and \(\cosh \lambda = \exp(|U| \Delta \tau / 2)\). For \(U < 0\), the special case of \(\mathbf{n} = \hat{z}\) is the familiar density (charge) decoupling scheme.

2. Auxiliary fields with enlarged manifold

When the manifold of auxiliary fields is larger than the minimal one, there will be some freedom in choosing the value of parameters in the HS transformation. An interesting such example for the Hubbard interactions was proposed by Hirsch [71] as follows:

\[
e^{-U \Delta \tau(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})} = \frac{b}{2} e^{-U \Delta \tau / 4} \sum_{s_{\uparrow}, s_{\downarrow} \in \{-1, 1\}} \exp(-\xi s_{\uparrow} s_{\downarrow} + \xi s_{\uparrow} (2n_{\uparrow} - 1) + s_{\downarrow} (2n_{\downarrow} - 1)),
\]

where \(\cosh(2\xi) = \frac{e^{U \Delta \tau / 2} - e^{-U \Delta \tau / 2}}{1 - e^{U \Delta \tau / 2} - e^{-U \Delta \tau / 2}}\) and \(b = \frac{1}{e^{U \Delta \tau / 2} - e^{-U \Delta \tau / 2}}\). Here \(\xi\) is not fixed and can be treated as a continuous parameter. In general, a HS transformation can be continuously parameterized by extending the value space or manifold of auxiliary fields. For the Hubbard interaction, another continuous parameterizations can be realized by extending the manifold from \(\{\pm 1\}\) to \(\{\pm n, \pm (n - 1), \cdots, \pm 1, 0\}\) as follows:

\[
e^{-U \Delta \tau(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})} = \sum_{s = \{\pm n, \pm (n - 1), \cdots, 0\}} \eta(s) e^{\lambda(s) s \hat{s}},
\]

where \(\eta(s) = \eta(-s)\) and \(\lambda(s) = \lambda(-s)\) which satisfy

\[
\sum_{s = \{\pm n, \pm (n - 1), \cdots, 0\}} \eta(s) = \exp(-U \Delta \tau / 4)
\]

\[
\sum_{s = \{\pm n, \pm (n - 1), \cdots, 0\}} \eta(s) \cosh(\lambda(s) s) = \exp(U \Delta \tau / 4).
\]

There are totally \(2(n + 1)\) parameters in the HS parameters, including \((n + 1)\) parameters \(\eta(s)\) and \((n + 1)\) parameters \(\lambda(s)\). However, there are only 2 constraints. It is clear that this kind of HS transformations can be continuous parameterized by \(2n\) parameters.

3. Hybrid HS transformations

When there are two or more different schemes of performing HS transformations for a certain type of interaction, one can introduce a hybrid HS transformation which can combine these schemes. For instance, suppose that there are two different HS schemes, one can split \(e^{-\Delta \tau \hat{H}_1}\) into two parts \(e^{-\Delta \tau_1 \hat{H}_1} e^{-\Delta \tau_2 \hat{H}_1}\), where \(\Delta \tau_1 + \Delta \tau_2 = \Delta \tau\), and then perform different HS transformations in each part:

\[
e^{-\Delta \tau \hat{H}_1} = \sum_{s_1, s_2} \eta_1(s_1) \eta_2(s_2) e^{\hat{V}_1(s_1)} e^{\hat{V}_2(s_2)},
\]
FIG. A1. Results of Hubbard-Rashba model on $3 \times 3$ honeycomb lattice with $\beta = 5, U = 6, t = 1.0, \Delta \tau = 0.1$ with periodic boundary condition. In each iteration, the gradients is average by 224 samples, where 224 is the number of paralleled Markov Chains. (a),(c): Optimization results for $\lambda_R = 1.5$ and $\lambda_R = 0.25$. (b),(d): Optimal pattern of $n$ for $\lambda_R = 1.0$ and $\lambda_R = 0.5$. Arrow represent the projection of $n$ in $xy$ plane. Here we use the equivalence relation $n \equiv -n$ to make $n_z > 0$. The optimal pattern of $\lambda_R = 1.5$ is still a AB sub-lattice pattern just like the case of $\lambda_R = 1.0$, while the optimal pattern of $\lambda_R = 0.25$ is like a stripe pattern.

where $s_1, s_2$ are auxiliary fields for the two different HS transformations. We can use $0 < \Delta \tau_1 < \Delta \tau$ as a continuous parameter and then the hybrid HS transformation can be continuously parameterized. This hybrid approach can also be combined with the former ways of extending HS transformations. Which type of HS transformations can give rise to better sign can be automatically selected by performing ADSM.

B. Detailed derivation of gradients

It is clear that the partition function $Z = \sum w(\xi, s)$ of a quantum system is independent with parameters $\xi$ in the HS transformation. As the average sign $S = \frac{\sum w(\xi, s)}{\sum w|w(\xi, s)|}$, the differentiation of $\ln S$ can be evaluated as

$$d\ln S = d\ln Z - d(\ln \sum_s |w(\xi, s)|) = -\left(\frac{dw(\xi, s)}{|w(\xi, s)|}\right)_{s \sim |w(\xi, s)|} = -\text{Re} \left(\frac{dw(\xi, s)}{|w(\xi, s)|}\right)_{s \sim |w(\xi, s)|},$$  \hspace{1cm} (A7)

where the last equality used the fact that $\text{Re} \frac{dw}{|w|} = \text{Re} (\frac{dw}{|w|} + id\varphi) = \frac{dw}{|w|}$. The reason why we don’t use the sign $S$ itself as target function becomes clearer using this result that $dS = S \times d\ln S$ will be very small if the sign problem is severe.

For the gauged HS transformation of the Hubbard interaction $\eta(\xi, s) = \frac{1}{2} e^{-U\Delta \tau/4}$, there is no dependence on the parameters $\xi$. Thus, it does not contribute the gradients:

$$\frac{dw}{w} = \sum_i \text{Tr} \left(\bar{G}_i(e^{K}e^{V(i)})^{-1}d(e^{K}e^{V(i)})\right) = \sum_i \text{Tr} \left(\bar{G}_i(e^{V(i)})^{-1}d(e^{V(i)})\right).$$  \hspace{1cm} (A8)

The last term in the gauged HS can be represented as:

$$(e^{V(i)})^{-1}d(e^{V(i)}) = U e^{-\lambda \sum \tau_i s_i \sigma_i} \sum \tau_i s_i \sigma_i d(\text{U} e^{\lambda \sum \tau_i s_i \sigma_i}) = \sinh(\lambda) \sum_i s_i \tau_i (\text{U} \sigma_x \tau_i \text{U})^d \theta_i + \text{U} \sigma_y \tau_i \text{U}^d \sin(\theta_i) d\phi_i,$$  \hspace{1cm} (A9)

where $\text{U} = \prod_i e^{-i \phi_i^{(s)}} e^{-i \phi_i^{(y)}}$. Then, we obtain explicit expressions for the gradients:

$$\frac{\partial \ln S}{\partial \theta_i} = -\sinh(\lambda) \text{Re} \left(\sum_l s_i \tau_l \text{Tr} \left[\bar{G}_l e^{-V(i)} \text{U} \sigma_x \tau_l \text{U}^d \theta_l + \text{U} \sigma_y \tau_l \text{U}^d \sin(\theta_l) d\phi_l\right]\right|_{|w|},$$  \hspace{1cm} (A10)

$$\frac{\partial \ln S}{\sin(\theta_i) \partial \phi_i} = -\sinh(\lambda) \text{Re} \left(\sum_l s_i \tau_l \text{Tr} \left[\bar{G}_l e^{-V(i)} \text{U} \sigma_x \tau_l \text{U}^d \theta_l + \text{U} \sigma_y \tau_l \text{U}^d \sin(\theta_l) d\phi_l\right]\right|_{|w|}.$$
C. Stabilization scheme of gradients calculation

In this work we use QR decomposition with column pivoting to stabilize the matrix cluster production encountered in the calculation of gradients and equal-time green function.

Algorithm 1: QRP stabilization

1) Compute pivoted QR: \( B_0 = QRP^T \)
2) set \( U_0 = Q, D_0 = \text{diag}(R), V_0 = D_0^{-1}RP^T \)
3) for \( i \) in range(1,L)
   \[ \text{Compute pivoted QR: } (B_iU_{i-1})D_{i-1} = QRP^T \]
   \[ \text{Set } U_i = Q, D_i = \text{diag}(R), V_i = D_i^{-1}RP^T V_{i-1} \]
end
4) Result: \( B_1B_0 \cdots B_0 = U_iD_iV_i \)

As shown in Alg. (1), matrix cluster production can be decomposed into \( UDV \), where \( U \) is a unitary matrix, \( D \) is a diagonal matrix and \( V \) is supposed to be a well-conditioned matrix. Applying this algorithm to the calculation of \( \bar{G}_l \), we get the decompositions:

\[
B_l \cdots B_1 = U_R D_R V_R \\
B_{L-1} \cdots B_1 = V_L D_L U_L
\] (A11)

It should be noticed that the second decomposition is in a reverse order \( VDU \) instead of \( UDV \) which can be easily realized by processing the matrixes from the left. The reason why we decompose these two productions into the above form is that these \( U_R, D_R, V_R, U_L, D_L, V_L \) are just by-products of the standard DQMC method since they are also necessary ingredients to stabilize the calculation of equal-time green functions needed for updating the auxiliary field configurations. No extra computational resources apart from some memory costs will be required to get these values. Using these results, \( \bar{G}_l \) can be calculated via a numerical stable routine:

\[
\bar{G}_l = (I + U_L^{-1}D_L^{-1}V_L^{-1}V_R^{-1}D_R^{-1}U_R^{-1})^{-1}U_R(U_L U_R + D_L^{-1}V_L^{-1}V_R^{-1}D_R^{-1})^{-1}U_L \\
= U_R D_R^b (D_L^b U_L U_R D_R^b + D_L^b V_L^{-1}V_R^{-1}D_R^{-1})^{-1}D_L^s U_L
\] (A12)

where \( D_{L,R} = D_{L,R}^b D_{L,R}^s \) and

\[
(D_{L,R}^b)_{ii} = \begin{cases} 
(D_{L,R})_{ii}, & \text{if } |(D_{L,R})_{ii}| > 1 \\
1, & \text{otherwise}
\end{cases}
\]

\[
(D_{L,R}^s)_{ii} = \begin{cases} 
1, & \text{if } |(D_{L,R})_{ii}| > 1 \\
(D_{L,R})_{ii}, & \text{otherwise}
\end{cases}
\] (A13)

The rounding error caused by the addition operation in Eq. (5) is eliminated by balancing the magnitude of the matrixes to add up.

FIG. A2. Optimal \( \theta \) value by restricting that \( \theta_B = -\theta_A = \theta, \phi_A = \phi_B = \pi/6 \). Noticing that there is a jump near \( \lambda_R = 0.5 \) which indicates that there may exist a transition of the pattern that the optimal pattern is not AB sublattice like. For example the hexagon pattern when \( \lambda_R = 0.5 \) or stripe pattern when \( \lambda_R = 0.25 \).
D. More results of different $\lambda_R$

In Fig. A1, we present the optimization results for $\lambda_R = 0.25$ and $\lambda_R = 1.5$. Here the optimal pattern of $n$ with $\lambda_R = 1.5$ is similar to the pattern of $\lambda_R = 1.0$ which has sub-lattice structure, while the optimal pattern of $\lambda_R = 0.25$ is stripe-like which is qualitatively different from $\lambda_R = 0.5, 1.0, 1.5$. By using constraints that $\theta_B = -\theta_A = \theta$, $\phi_A = \phi_B = \pi/6$, we find the optimized $\theta_{opt}$ with different $\lambda_R$. The results are shown in Fig. A2. Clearly, optimal patterns of $\lambda_R = 0.5, 0.25$ violate these constraints. As a result, we found that there is a jump of $\theta_{opt}$ near $\lambda = 0.5$ which indicates a pattern transition in this parameter region.