DQMC Notes

Jixun K. Ding

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1 Hubbard-Stratonovich transformations

Auxiliary field QMC methods are based on various forms of the **Hubbard-Stratonovich (HS) transformation**. A HS transformation converts a particle theory into its respective field theory by linearizing the density operator in the many-body interaction term of the Hamiltonian and introducing an auxiliary scalar field. This transformation is *not unique*. The efficiency of the QMC algorithm depends substantially on the type of HS transformation one uses.
A generic HS transformation relies on the following Gaussian integral identities for real variables (or classical scalar fields) $x \in \mathbb{R}$ (these identities are sometimes themselves called HS transformations):

- 1-D Gaussian integral. $a > 0$:

$$\int dx \exp\left[-\frac{1}{2}ax^2\right] = \sqrt{\frac{2\pi}{a}} \tag{1.1}$$

- 1-D Gaussian integral with real linear term. $a > 0$, $J \in \mathbb{R}$:

$$\int dx \exp\left[-\frac{1}{2}ax^2 \pm Jx\right] = \sqrt{\frac{2\pi}{a}} \exp\left[\frac{J^2}{2a}\right] \tag{1.2}$$

$$\int dx \exp\left[-\frac{1}{2a}x^2 \pm Jx\right] = \sqrt{2\pi a} \exp\left[\frac{a}{2}J^2\right] \tag{1.3}$$

- 1-D Gaussian integral with imaginary linear term. $a > 0$, $J \in \mathbb{R}$ [contour integral in complex plane]:

$$\int dx \exp\left[-\frac{1}{2}ax^2 \pm iJx\right] = \sqrt{\frac{2\pi}{a}} \exp\left[\frac{-J^2}{2a}\right] \tag{1.4}$$

$$\int_{-\infty}^{\infty} dx \exp\left[-\frac{1}{2a}x^2 \pm iJx\right] = \sqrt{2\pi a} \exp\left[-\frac{a}{2}J^2\right] \tag{1.5}$$

In particular, consider an identity of the form Eq. (1.3), but let J be a *fermionic* one-body operator. Then what the identity says is that we may transform the two-body operator $\exp[J^2]$ into the an integral of the one-body operator J interacting with the bosonic field x. The key is that for a fixed field x, the one-body fermion problem is exactly solvable. The integral over the field x can then be carried out with e.g. Monte Carlo methods [FSW08].
The following subsections consider some simple examples of HS transformations.

1.1 Repulsive, purely local Hubbard interaction

The local Hubbard interaction term for a site i is

$$V_i = U_i(n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) = -\frac{U_i}{2}(n_{i\uparrow} - n_{i\downarrow})^2 + \frac{U_i}{4} \tag{1.6}$$

and we want to compute $\exp[-\Delta\tau V_i]$ (e.g. in Eq. (2.4)), which can be accomplished by writing $J = n_{i\uparrow} - n_{i\downarrow}$, and finding [c.f. Eq. (1.3)]

$$\exp\left[\frac{+\Delta\tau U_i}{2}(n_{i\uparrow} - n_{i\downarrow})^2\right] = \frac{1}{\sqrt{2\pi(\Delta\tau U_i)}}\int_{-\infty}^{\infty} dx \exp\left[-\frac{1}{2(\Delta\tau U_i)}x^2 \pm (n_{i\uparrow} - n_{i\downarrow})x\right], \tag{1.7}$$

and performing the RHS integral via e.g. Monte Carlo sampling over x. However, Monte Carlo integration over a continuous field is cumbersome, and we'd much rather be summing over a discrete field. Noticing that the Hilbert space for a single site consists of only four states, we propose the identity (assuming $U_i > 0$ is repulsive)

$$\exp[-\Delta\tau V_i] = \gamma \sum_{x=\pm 1} \exp[\lambda x(n_{i\uparrow} - n_{i\downarrow})] \tag{1.8}$$

and look for values of λ and γ to satisfy the identity Eq. (1.8) for all 4 possible local states. This is accomplished by

$$\gamma = \frac{1}{2}\exp\left[-\Delta\tau U_i/4\right], \quad \lambda = \cosh^{-1}\exp[+\Delta\tau U_i/2] \tag{1.9}$$

This choice of HS transformation leads to an efficient Monte Carlo algorithm for repulsive Hubbard type models. However, as written, Eq. (1.9) breaks SU(2) spin symmetry. Since the HS field x couples to the z-component of the magnetization, the spin symmetry is broken for any fixed value of the field x, and is restored only after summation over the field. To avoid this symmetry breaking, we may consider an alternative HS decomposition by noting the local Hubbard interaction can also be written as

$$V_i = U_i(n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) = \frac{U_i}{2}(n_{i\uparrow} + n_{i\downarrow} - 1)^2 - \frac{U_i}{4} \tag{1.10}$$

which allows $n_{i\uparrow} + n_{i\downarrow} - 1$ to play the role of J. Analogous to Eq. (1.8), we instead posit that (assuming $U_i > 0$ is repulsive)

$$\exp[-\Delta\tau V_i] = \gamma \sum_{x=\pm 1} \exp[i\lambda x(n_{i\uparrow} + n_{i\downarrow} - 1)], \tag{1.11}$$

and find that Eq. (1.11) can be satisfied by

$$\gamma = \frac{1}{2}\exp\left[+\Delta\tau U_i/4\right], \quad \lambda = \cos^{-1}\exp[-\Delta\tau U_i/2]. \tag{1.12}$$

However, in maintaining explicit SU(2) symmetry for every realization of field x, this decomposition requires us to work with complex numbers. Inserting an i in to the exponent of the RHS of Eq. (1.11) is necessary when $U_i > 0$ so we can find a solution for λ.

1.2 Attractive, purely local Hubbard interaction

When $U_i < 0$ is attractive, the situation is analogous to Eq. (1.11) but actually even simpler. We posit that

$$\exp[-\Delta\tau V_i] = \gamma \sum_{x=\pm 1} \exp[\lambda x(n_{i\uparrow} + n_{i\downarrow} - 1)], \tag{1.13}$$

which we find can be satisfied by something which looks very similar to Eq. (1.9):

$$\gamma = \frac{1}{2}\exp\left[+\Delta\tau U_i/4\right] = \frac{1}{2}\exp\left[-\Delta\tau|U_i|/4\right], \quad \lambda = \cosh^{-1}\exp[+\Delta\tau|U_i|/2]. \tag{1.14}$$

Note this decomposition does not require the use of complex numbers.

In Eq. (1.8), the discrete HS field x couples to the z-axis magnetization $n_{i\uparrow} - n_{i\downarrow}$, while in Eqs. (1.11) and (1.13), the discrete HS field x couples to particle density $n_{i\uparrow} + n_{i\downarrow} - 1$.

2 Description of DQMC

In general, attempts to exactly solve interacting Hamiltonians suffer from exponential scaling of the size of the Hilbert space with the number of particles or the size of the system. If there are c states per particle, and N_e particles, then the dimension of the interacting Hilbert space scales as $|\mathcal{H}| = c^{N_e}$, compared to the non-interacting case $|\mathcal{H}| = cN_e$. It's not possible to design a general-purpose classical (in that it runs on classical, not quantum, computers) algorithm that solves (in that we obtain all eigenstates and eigenvalues) exponential problems in polynomial time. However, not all hope is lost. It's possible to be clever and design polynomial-time algorithms for 1) restricted classes of Hamiltonians that 2) don't produce complete information about the system, only physically measurable observables. Determinant quantum Monte Carlo (DQMC) is one example of such an algorithm.
DQMC considers interacting lattice fermion Hamiltonians of the form

$$H = K + V = K + \sum_i V_i \tag{2.1}$$

where K is a non-interacting kinetic term that incorporates the chemical potential, and V is the interaction term which decomposes into a sum of local interactions V_i. The goal is to compute thermal expectation values (in the grand canonical ensemble) of arbitrary operator O at inverse temperature $\beta = 1/(k_B T)$

$$\langle O\rangle = \frac{\mathrm{Tr}\left[O\exp(-\beta H)\right]}{\mathcal{Z}} = \frac{\mathrm{Tr}\left[O\exp(-\beta H)\right]}{\mathrm{Tr}\left[\exp(-\beta H)\right]}. \tag{2.2}$$

In order to do so, let's first discretize imaginary time into L slices of width $\Delta\tau$, $\beta = L\Delta\tau$, and apply the Suzuki–Trotter decomposition. The partition function becomes

$$\mathcal{Z} \approx \mathrm{Tr}\left[\prod_{l=0}^{L-1}\exp[-\Delta\tau K]\exp[-\Delta\tau V]\right] = \mathrm{Tr}\left[\prod_{l=0}^{L-1}\exp[-\Delta\tau K]\exp\left[-\Delta\tau\sum_{i=0}^{N-1}V_i\right]\right] \tag{2.3}$$

$$= \mathrm{Tr}\left[\prod_{l=0}^{L-1}\exp[-\Delta\tau K]\prod_{i=0}^{N-1}\exp\left[-\Delta\tau V_i\right]\right]. \tag{2.4}$$

Note that as $[K, V] \neq 0$, terms at different imaginary time slices labelled by l do not commute with each other.

For the Hubbard model,

$$K = K_\uparrow + K_\downarrow = c^\dagger_{i\uparrow}k_{\uparrow ij}c_{j\uparrow} + c^\dagger_{i\downarrow}k_{\downarrow ij}c_{j\downarrow} = \mathbf{c}^\dagger_\uparrow k_\uparrow \mathbf{c}_\uparrow + \mathbf{c}^\dagger_\downarrow k_\downarrow \mathbf{c}_\downarrow \tag{2.5}$$

where each $\mathbf{c}_{\uparrow/\downarrow}$ is a length N vector of fermion operators, and $k_{\uparrow/\downarrow}$ is a $N \times N$ ordinary matrix of complex numbers.

Let's say for simplicity that we are dealing with repulsive, purely local Hubbard interaction terms, Eq. (1.6) with $U_i > 0$. To decouple these interaction terms, we apply independent discrete Hubbard-Stratonovich transformations Eq. (1.8) at each imaginary time slice l and lattice site i. Changing notation $x \to s_{il}$ to capture this dependence, and additionally assuming $U_i = U, \forall i$, we find that after plugging Eqs. (1.8) and (2.5) into Eq. (2.4), the partition function becomes (N is the total number of lattice sites)

$$\begin{aligned}
\mathcal{Z} &= \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \prod_{i=0}^{N-1} \exp\left[-\Delta\tau U_i/4\right] \frac{1}{2} \sum_{s_{il}=\pm 1} \exp[\lambda s_{il}(n_{i\uparrow}-n_{i\downarrow})]\right] \\
&= 2^{-NL}\exp[-\beta N U]\mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \prod_{i=0}^{N-1} \sum_{s_{il}=\pm 1} \exp[\lambda s_{il}(n_{i\uparrow}-n_{i\downarrow})]\right] \\
&\propto \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \sum_{\mathbf{s}_l=\{\pm 1\}^N} \exp\left[\lambda \sum_{i=0}^{N-1} s_{il}(n_{i\uparrow}-n_{i\downarrow})\right]\right] \\
&= \sum_{\mathbf{s}=\{\pm 1\}^{NL}} \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp\left[\lambda \sum_{i=0}^{N-1} s_{il} n_{i\uparrow}\right]\exp[-\Delta\tau K_\downarrow]\exp\left[-\lambda \sum_{i=0}^{N-1} s_{il} n_{i\downarrow}\right]\right] \\
&= \sum_{\mathbf{s}=\{\pm 1\}^{NL}} \mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\uparrow(\mathbf{s}) D_l^\downarrow(\mathbf{s})\right] = \sum_{\mathbf{s}=\{\pm 1\}^{NL}} \mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\uparrow(\mathbf{s})\right] \mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\downarrow(\mathbf{s})\right],
\end{aligned} \tag{2.6}$$

where we have denoted

$$D_l^\uparrow(\mathbf{s}) = \exp[-\Delta\tau K_\uparrow]\exp\left[\lambda \sum_{i=0}^{N-1} s_{il} n_{i\uparrow}\right] \tag{2.7}$$

$$D_l^\downarrow(\mathbf{s}) = \exp[-\Delta\tau K_\downarrow]\exp\left[-\lambda \sum_{i=0}^{N-1} s_{il} n_{i\downarrow}\right] \tag{2.8}$$

and noticed that $D_l^\uparrow(D_l^\downarrow)$ only involve $c_\uparrow(c_\downarrow)$ operators, so the fermionic trace can be decomposed as $\mathrm{Tr}\left[A \otimes B\right] = \mathrm{Tr}\left[A\right]\mathrm{Tr}\left[B\right]$.
At this point, we have decoupled the interaction by introducing a sum over all configurations of a real-space imaginary-time auxiliary field $\mathbf{s} = \{s_{il}\} \in \{\pm 1\}^{NL}$. The problem becomes one of *free* fermions interacting with a fluctuating Ising spin field. Since the matrices $D_l^\uparrow(D_l^\downarrow)$ only involve quadratic forms of fermion operators, the integration/trace over fermionic degrees of freedom can be taken exactly by using the identities [BSS81]

$$\mathrm{Tr}\left[\prod_l \exp[H_l]\right] = \det\left[I + \prod_l \exp[h_l]\right] = \det(M) \tag{2.9}$$

$$\left(M^{-1}\right)_{ij} = g_{ij} = \langle c_i c_j^\dagger \rangle \tag{2.10}$$

where $H_l = \mathbf{c}^\dagger h_l \mathbf{c}$, and h_l, M, g are ordinary $N \times N$ matrices.
After plugging Eqs. (2.9) and (2.10) into Eq. (2.6), we find the partition function is written in terms of a sum over the product of weights for each fermionic flavor,

$$Z \propto \sum_{\mathbf{s}} w(\mathbf{s}) = \sum_{\mathbf{s}} w^\uparrow(\mathbf{s}) w^\downarrow(\mathbf{s}) = \sum_{\mathbf{s}} \det\left(M^\uparrow(\mathbf{s})\right) \det\left(M^\downarrow(\mathbf{s})\right) \tag{2.11}$$

where

$$M^\uparrow(\mathbf{s}) = I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_\uparrow + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right] = (g^\uparrow)^{-1} \tag{2.12}$$

$$M^\downarrow(\mathbf{s}) = I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_\downarrow - \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right] = (g^\downarrow)^{-1} \tag{2.13}$$

Instead of solving for all configurations $\mathbf{s}$, the DQMC algorithm proceeds by performing importance sampling (with standard Monte Carlo techniques) over $\mathbf{s}$ by interpreting the configuration-dependent Boltzmann weight $|w(\mathbf{s})|$ as a probability distribution. It's necessary to use the absolute value, because in general, $w(\mathbf{s})$ may be negative [c.f. Section 3]. Assuming that the importance sampling is converged, then

$$\begin{aligned}\langle O\rangle \approx \langle O\rangle_{\mathrm{MC},w(\mathbf{s})} &= \frac{\sum_s O_{\mathbf{s}} w_{\mathbf{s}}}{\sum_s w_{\mathbf{s}}} = \frac{\sum_s O_{\mathbf{s}}|w_{\mathbf{s}}|\mathrm{sgn}(w_{\mathbf{s}})}{\sum_s |w_{\mathbf{s}}|\mathrm{sgn}(w_{\mathbf{s}})} = \frac{\sum_s O_{\mathbf{s}}|w_{\mathbf{s}}|\mathrm{sgn}(w_{\mathbf{s}})/\sum_s |w_{\mathbf{s}}|}{\sum_s |w_{\mathbf{s}}|\mathrm{sgn}(w_{\mathbf{s}})/\sum_s |w_{\mathbf{s}}|} \\ &= \frac{\langle O\mathrm{sgn}(w_{\mathbf{s}})\rangle_{\mathrm{MC},|w(\mathbf{s})|}}{\langle \mathrm{sgn}(w_{\mathbf{s}})\rangle_{\mathrm{MC},|w(\mathbf{s})|}} \equiv \frac{\langle Os\rangle_{\mathrm{MC},|w(\mathbf{s})|}}{\langle s\rangle_{\mathrm{MC},|w(\mathbf{s})|}}\end{aligned} \tag{2.14}$$

The single, controllable approximation used in the DQMC algorithm is the imaginary-time discretization interval $\Delta\tau$, which introduces an error of size $O\left((\Delta\tau)^2 tU\right)$.

2.1 Attractive Hubbard model

If instead, we are dealing with an attractive Hubbard model, with local $U_i < 0$, then the appropriate HS transformation to use is Eq. (1.13). Plugging Eqs. (1.13) and (2.5) into Eq. (2.4), the partition function becomes (assuming $U_i = U, \forall i$, and changing notation $x \to s_{il}$):

$$\begin{aligned}\mathcal{Z} &= \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \prod_{i=0}^{N-1} \exp\left[-\Delta\tau|U_i|/4\right]\frac{1}{2}\sum_{s_{il}=\pm 1}\exp[\lambda s_{il}(n_{i\uparrow}+n_{i\downarrow}-1)]\right] \\ &= 2^{-NL}\exp[-\beta N|U|]\mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \prod_{i=0}^{N-1}\sum_{s_{il}=\pm 1}\exp[\lambda s_{il}(n_{i\uparrow}+n_{i\downarrow}-1)]\right] \\ &\propto \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp[-\Delta\tau K_\downarrow] \sum_{\mathbf{s}_l=\{\pm 1\}^N}\exp\left[\lambda\sum_{i=0}^{N-1} s_{il}(n_{i\uparrow}+n_{i\downarrow}-1)\right]\right] \\ = \sum_{\mathbf{s}=\{\pm 1\}^{NL}} \mathrm{Tr}&\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow]\exp\left[\lambda\sum_{i=0}^{N-1} s_{il}n_{i\uparrow}\right]\exp[-\Delta\tau K_\downarrow]\exp\left[+\lambda\sum_{i=0}^{N-1} s_{il}n_{i\downarrow}\right]\exp\left[-\lambda\sum_i s_{il}\right]\right] \\ &= \sum_{\mathbf{s}=\{\pm 1\}^{NL}}\exp\left[-\lambda\sum_{il} s_{il}\right]\mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\uparrow(\mathbf{s})D_l^\downarrow(\mathbf{s})\right] \\ &= \sum_{\mathbf{s}=\{\pm 1\}^{NL}}\exp\left[-\lambda\sum_{il} s_{il}\right]\mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\uparrow(\mathbf{s})\right]\mathrm{Tr}\left[\prod_{l=0}^{L-1} D_l^\downarrow(\mathbf{s})\right]\end{aligned} \tag{2.15}$$

where we have denoted:

$$D_l^\uparrow(\mathbf{s}) = \exp[-\Delta\tau K_\uparrow]\exp\left[\lambda\sum_{i=0}^{N-1} s_{il}n_{i\uparrow}\right] \tag{2.16}$$

$$D_l^\downarrow(\mathbf{s}) = \exp[-\Delta\tau K_\downarrow]\exp\left[\lambda\sum_{i=0}^{N-1} s_{il}n_{i\downarrow}\right] \tag{2.17}$$

and noticed that $D_l^\uparrow(D_l^\downarrow)$ only involve $c_\uparrow(c_\downarrow)$ operators, so the fermionic trace can be decomposed as $\mathrm{Tr}\left[A\otimes B\right] = \mathrm{Tr}\left[A\right]\mathrm{Tr}\left[B\right]$.
After plugging Eqs. (2.9) and (2.10) into Eq. (2.15), we find the partition function is written in terms of a sum over the product of weights for each fermionic flavor,

$$Z \propto \sum_{\mathbf{s}} w(\mathbf{s}) = \sum_{\mathbf{s}} e^{-\lambda\sum_{il} s_{il}} w^\uparrow(\mathbf{s})w^\downarrow(\mathbf{s}) = \sum_{\mathbf{s}} e^{-\lambda\sum_{il} s_{il}}\det\left(M^\uparrow(\mathbf{s})\right)\det\left(M^\downarrow(\mathbf{s})\right) \tag{2.18}$$

where

$$M^{\uparrow}(\mathbf{s}) = I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_{\uparrow} + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right] = (g^{\uparrow})^{-1} \tag{2.19}$$

$$M^{\downarrow}(\mathbf{s}) = I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_{\downarrow} + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right] = (g^{\downarrow})^{-1} \tag{2.20}$$

3 Sign problem

There is no free lunch, and the hidden "gotcha" of the DQMC algorithm lies in the fermion sign problem, i.e. the fact that the weights $w_{\mathbf{s}}$ are not always positive semi-definite [LGS+90]. This can be fundamentally attributed to negative signs introduced by braiding fermion world lines [IST16]. For most generic models, parameters, lattices, and choice of Hubbard-Stratonovich decomposition (or more generally, bosonization procedure), the DQMC simulation is "sign-problem-full." What's worse, the fermion sign problem is exponentially bad, in the sense that if system size is N and inverse temperature is β, then the average sign $\langle s \rangle$ exponentially decays as

$$\langle s \rangle \propto \exp[-(\#)N] \quad \text{and} \quad \langle s \rangle \propto \exp[-(\#)\beta] \tag{3.1}$$

for sufficiently large lattice size and sufficiently low temperature (see [IKS15] for some examples).
When the average sign $\langle s \rangle$ is small, applying Eq. (2.14) will

- Introduce bias. Assuming $\langle Os \rangle_{\mathrm{MC},|w(\mathbf{s})|}$ and $\langle s \rangle_{\mathrm{MC},|w(\mathbf{s})|}$ are each individually normally distributed, their ratio is not necessarily normally distributed. In pratice, we always correct for this bias using jackknife or bootstrap resampling.
- Amplify statistical fluctuations. To acquire meaningful information from a Monte Carlo algorithm, we need to average over a large enough number N_s of configurations s to obtain an expectation value $\langle A \rangle$ with some relative statistical error $\epsilon = \sigma_A / \langle A \rangle$, where ϵ is small. However, as $\langle s \rangle$ becomes exponentially small, its relative error $\sigma_s / \langle s \rangle$ blows up, which means the number of samples one must acquire to reach the desired error tolerance also grows exponentially [TW05].

Due to the second point, the exponentially bad fermion sign problem prevents us from obtaining informative simulation data in many cases of physical interest.
It's important to note that the fermion sign is a property of both the model Hamiltonian and the representation we choose to simulate it. A given model Hamiltonian may not admit a sign-free representation, and if a model does admit a sign-free representation, it's not guaranteed that we are clever enough to find it. As the fermion sign problem is believed to be NP-hard [TW05], we don't expect a general "solution" to the fermion sign problem to exist. Nevertheless, it is possible to reduce or completely remove the sign problem for DQMC simulations of some classes of non-generic Hamiltonians [WZ05, LJY15].
On the other hand, once we fix the simulation scheme, e.g. to be of DQMC type, then we find the presence and severity of the fermion sign problem are correlated with physical properties of a model Hamiltonian. Some results of this kind include

- Ref. [GB23]: a model belonging to any of the known sign-free classes within DQMC cannot have a stable Fermi-liquid ground state in spatial dimension $d \geq 2$.
- Ref. [GSR20]: "most" gapped chiral topological phases of matter do not have sign-free model Hamiltonians within DQMC.
- Ref. [MTS22]: qualitatively, the sign problem is often exacerbated near quantum critical points.

3.1 Sign-free examples

Claim 3.1. The attractive Hubbard model in any lattice geometry with possibly complex kinetic matrices is sign-problem-free.

Proof. by inspecting Eq. (2.18), we see that if $k_\uparrow = k_\downarrow^*$ (so the system overall is time-reversal symmetric), then we have $M^\uparrow(\mathbf{s})^* = M^\downarrow(\mathbf{s})$, so $w(\mathbf{s}) \geq 0$ for all $\mathbf{s}$. ∎

On the other hand, if $k_\uparrow = k_\downarrow$ (so the system overall may break time-reversal symmetry), then in general, $M^\uparrow(\mathbf{s})^* \neq M^\uparrow(\mathbf{s}) = M^\downarrow(\mathbf{s})$. Adding a Zeeman field, i.e. spin-dependent chemical potential terms, also introduces a sign problem.

Claim 3.2. The $t' = 0$ repulsive Hubbard model

$$\begin{aligned} H &= -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \\ &= \mathbf{c}_\uparrow^\dagger (h_\uparrow - \mathrm{diag}(\mu)) \mathbf{c}_\uparrow + \mathbf{c}_\downarrow^\dagger (h_\downarrow - \mathrm{diag}(\mu)) \mathbf{c}_\downarrow + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \end{aligned} \tag{3.2}$$

on a bipartite lattice at half-filling ($\mu = 0$) is sign-problem-free.

Proof. Consider a *unitary* half particle-hole transformation, acting only on the spin-down electrons

$$c_{i\downarrow} \to d_{i\downarrow} = (-1)^i c_{i\downarrow}^\dagger, \quad c_{i\downarrow}^\dagger \to d_{i\downarrow}^\dagger = (-1)^i c_{i\downarrow}, \tag{3.3}$$

where $(-1)^i$ is not literal but means $+1$ on sublattice A and -1 on sublattice B.
Denoting $\tilde{n}_{i\downarrow} = d_{i\downarrow}^\dagger d_{i\downarrow}$, we find $n_{i\sigma} = 1 - \tilde{n}_{i\sigma}$, and for nearest neighbor pairs $\langle ij \rangle$,

$$d_{i\downarrow}^\dagger d_{j\downarrow} = c_{j\downarrow}^\dagger c_{i\downarrow}, \quad d_{j\downarrow}^\dagger d_{i\downarrow} = c_{i\downarrow}^\dagger c_{j\downarrow}, \tag{3.4}$$

we can re-write the Hubbard Hamiltonian as

$$H = \mathbf{c}_\uparrow^\dagger \left(h_\uparrow - \mathrm{diag}(\mu)\right) \mathbf{c}_\uparrow + \mathbf{d}_\downarrow^\dagger \left(h_\downarrow + \mathrm{diag}(\mu)\right) \mathbf{d}_\downarrow - U \sum_i (n_{i\uparrow} - 1/2)(\tilde{n}_{i\downarrow} - 1/2), \tag{3.5}$$

which can be decomposed as an attractive Hubbard model, per Section 2.1

$$\mathcal{Z} \propto \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow] \exp[-\Delta\tau K_\downarrow] \sum_{\mathbf{s}_l = \{\pm 1\}^N} \exp\left[\lambda \sum_{i=0}^{N-1} s_{il}(n_{i\uparrow} + \tilde{n}_{i\downarrow} - 1)\right]\right] \tag{3.6}$$

$$= \sum_{\mathbf{s}} \exp\left[-\lambda \sum_{il} s_{il}\right] \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K_\uparrow] \exp\left[\lambda \sum_{i=0}^{N-1} s_{il} n_{i\uparrow}\right] \exp[-\Delta\tau K_\downarrow] \exp\left[\lambda \sum_{i=0}^{N-1} s_{il} \tilde{n}_{i\downarrow}\right]\right] \tag{3.7}$$

$$= \sum_{\mathbf{s}} e^{-\lambda \sum_{il} s_{il}} \det\left[I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_\uparrow + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right]\right] \det\left[I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_\downarrow + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right]\right]. \tag{3.8}$$

By inspecting Eq. (3.5) we see when $\mu = 0$, the kinetic matrices $k_\uparrow, k_\downarrow$ are equal and entirely real, so $w(\mathbf{s}) \geq 0$ for all $\mathbf{s}$. ∎

Proof. The following argument can be found in Ref. [Hir85]. Consider applying the half particle-hole transform Eq. (3.3) directly to $w^\downarrow(\mathbf{s})$. When $\mu = 0$,

$$w^\downarrow(\mathbf{s}) = \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{c}_\downarrow^\dagger k_\downarrow \mathbf{c}_\downarrow] \exp\left[-\lambda \sum_{i=0}^{N-1} s_{il} n_{i\downarrow}\right]\right] \tag{3.9}$$

$$= \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{d}_\downarrow^\dagger k_\downarrow \mathbf{d}_\downarrow] \exp\left[+\lambda \sum_{i=0}^{N-1} s_{il} \tilde{n}_{i\downarrow}\right] \exp\left[\lambda \sum_{i=0}^{N-1} s_{il}\right]\right] \tag{3.10}$$

$$= \exp\left[\lambda \sum_{il} s_{il}\right] \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{d}^\dagger k_\downarrow \mathbf{d}] \exp\left[+\lambda \sum_{i=0}^{N-1} s_{il} \tilde{n}_{i\downarrow}\right]\right] \tag{3.11}$$

$$= \exp\left[\lambda \sum_{il} s_{il}\right] \det\left[I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k_\uparrow + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right]\right] = \exp\left[\lambda \sum_{il} s_{il}\right] w^\uparrow(\mathbf{s}) \tag{3.12}$$

where in the last line we also used $k_\uparrow = k_\downarrow$ and Eq. (2.12). This relation between $w^\uparrow(\mathbf{s})$ and $w^\downarrow(\mathbf{s})$ ensures that their product $w(\mathbf{s})$ is positive semi-definite. ■

Claim 3.3. The repulsive Hubbard-Hofstadter model

$$\begin{aligned} H = -t \sum_{\langle ij\rangle\sigma} \exp[i\varphi_{ij}] c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i \left(n_{i\uparrow} - 1/2\right)\left(n_{i\downarrow} - 1/2\right) \\ = \mathbf{c}^\dagger_\uparrow (h_\uparrow - \mathrm{diag}(\mu))\mathbf{c}_\uparrow + \mathbf{c}^\dagger_\downarrow (h_\downarrow - \mathrm{diag}(\mu))\mathbf{c}_\downarrow + U \sum_i \left(n_{i\uparrow} - 1/2\right)\left(n_{i\downarrow} - 1/2\right) \end{aligned} \tag{3.13}$$

on a bipartite lattice at half-filling ($\mu = 0$) is sign-problem-free.

Proof. Consider again Eq. (3.3). On a bipartite lattice, the Hubbard-Hofstadter Hamiltonian is re-written as

$$H = \mathbf{c}^\dagger_\uparrow \left(h_\uparrow - \mathrm{diag}(\mu)\right) \mathbf{c}_\uparrow + \mathbf{d}^\dagger_\downarrow \left(h^*_\downarrow + \mathrm{diag}(\mu)\right) \mathbf{d}_\downarrow - U \sum_i \left(n_{i\uparrow} - 1/2\right)\left(\tilde{n}_{i\downarrow} - 1/2\right), \tag{3.14}$$

which can be decomposed as an attractive Hubbard model, etc. Alternatively, apply the half particle-hole transform Eq. (3.3) directly to $w^\uparrow(\mathbf{s})$. When $\mu = 0$,

$$w^\downarrow(\mathbf{s}) = \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{c}^\dagger_\downarrow k_\downarrow \mathbf{c}_\downarrow] \exp\left[-\lambda \sum_{i=0}^{N-1} s_{il} n_{i\downarrow}\right]\right] \tag{3.15}$$

$$= \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{d}^\dagger_\downarrow k^*_\downarrow \mathbf{d}_\downarrow] \exp\left[+\lambda \sum_{i=0}^{N-1} s_{il} \tilde{n}_{i\downarrow}\right] \exp\left[\lambda \sum_{i=0}^{N-1} s_{il}\right]\right] \tag{3.16}$$

$$= \exp\left[\lambda \sum_{il} s_{il}\right] \mathrm{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{d}^\dagger_\downarrow k^*_\downarrow \mathbf{d}_\downarrow] \exp\left[+\lambda \sum_{i=0}^{N-1} s_{il} \tilde{n}_{i\downarrow}\right]\right] \tag{3.17}$$

$$= \exp\left[\lambda \sum_{il} s_{il}\right] \det\left[I + \prod_{l=0}^{L-1} \exp\left[-\Delta\tau k^*_\uparrow + \lambda \cdot \mathrm{diag}(\mathbf{s}_l)\right]\right] = \exp\left[\lambda \sum_{il} s_{il}\right] \left(w^\uparrow(\mathbf{s})\right)^* \tag{3.18}$$

where in the last line we also used $k_\uparrow = k_\downarrow$ and Eq. (2.12). This relation between $w^\uparrow(\mathbf{s})$ and $w^\downarrow(\mathbf{s})$ again ensures that their product $w(\mathbf{s})$ is positive semi-definite. ■

In the examples above, we relied on the "factorizability" of the fermion determinant $w(\mathbf{s})$ into spin-up and spin-down components. But for more complicated models, the fermion determinants may not be factorizable. The good news is that we actually don't need factorizability of the fermion determinant to prove sign-free-ness. The following subsection discusses one class of Hamiltonians (the so called Kramers' class) for which one can prove that $w(\mathbf{s})$ is positive semi-definite so that the DQMC simulation is sign-problem-free.

3.2 Kramers' class of sign-free models

Ref. [WZ05] proposed the following principle for sign-free DQMC simulation:

Theorem 3.1. *For a set of square matrices H_l, if there exists an* antiunitary *operator T with $T^2 = -1$ such that $TH_lT^{-1} = H, \forall l$, then the eigenvalues of the matrix $M = 1 + \prod_l \exp[h_l]$ [c.f. Eq. (2.9)] always appear in complex conjugate pairs. Furthermore, $\det(M) = \prod_n |\lambda_n|^2 \geq 0$.*

This theorem can be understood as a generalization of the Kramers' doubling theorem:

Theorem 3.2 (Kramers' doubling theorem)**.** *Whenever we have a time-reversal symmetric (TRS) Hamiltonian, i.e. $[H, T] = 0$, and $T^2 = -1$ (i.e. we have half-integer spin, i.e. odd number of fermions), every energy level must be* ***at least*** *doubly (but more generally, can be fourfold, sixfold...etc) denegerate.*

If $1+\prod_l \exp[h_l]$ is Hermitian, then Theorem 3.1 reduces to Kramers' theorem, as the eigenvalues of $1+\prod_l \exp[h_l]$ are real and twofold degenerate.
A good example that uses Theorem 3.1 to demonstrate a model Hamiltonian is sign-free can be found in Ref. [HCH+20], where the authors consider a model that is equivalent to a two-orbital Hubbard model with on-site interspin repulsion and intra-orbital attraction ($\alpha \in A, B$; $U, V > 0$):

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{3.19}$$

$$\hat{H}_0 = -t \sum_{\langle i,j\rangle,\alpha,\sigma} \left(\hat{c}^\dagger_{i\alpha\sigma} \hat{\sigma}_{j\alpha\sigma} + \text{ H.c. } \right) - \mu \sum_{i\sigma} (\hat{n}_{iA\sigma} + \hat{n}_{iB\sigma}) \equiv K, \tag{3.20}$$

$$\hat{V} = U \sum_{i\alpha} \left(\hat{n}_{i\alpha\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\alpha\downarrow} - \frac{1}{2} \right) - V \sum_{i\sigma\sigma'} \left(\hat{n}_{iA\sigma} - \frac{1}{2} \right) \left(\hat{n}_{iB\sigma'} - \frac{1}{2} \right) = \sum_i \hat{V}_i, \tag{3.21}$$

After re-writing the interaction term as

$$\hat{V}_i = \frac{U-V}{4} (\hat{N}_i - 2)^2 + \frac{U+V}{4} \hat{M}_i^2 \tag{3.22}$$

where

$$\hat{N}_i = \sum_{\alpha\sigma} n_{i\alpha\sigma}, \quad \hat{M}_i = \sum_{\sigma} (\hat{n}_{iA\sigma} - \hat{n}_{iB\sigma}) \tag{3.23}$$

the local interaction term V_i is decomposed as

$$\exp[-\Delta\tau \hat{V}_i] = \sum_{s\in\{0,\pm1\}} \gamma_s \exp\left[\lambda s (\hat{N}_i - 2)\right] \sum_{s'\in\{0,\pm1\}} \gamma_{s'} \exp\left[\lambda' s' \hat{M}_i\right] \tag{3.24}$$

where the parameters $\gamma_s, \lambda, \gamma_{s'}, \lambda'$ are set by

$$\lambda(a) = \operatorname{arccosh}\left[\frac{1}{2} \left(e^{-3a} + e^{-2a} + e^{-a} - 1 \right) \right] \tag{3.25}$$

$$\gamma_0(a) = \frac{1 + \cosh(a)}{1 + 2\cosh(a) + \sinh(a)} \tag{3.26}$$

$$\gamma_{\pm1}(a) = \frac{1}{3 + e^{-2a} + 2e^{-a}} \tag{3.27}$$

where $a = \Delta\tau(U-V)/4$ for s, γ_s, λ; $a = \Delta\tau(U+V)/4$ for $s', \gamma_{s'}, \lambda'$, respectively. This transforms the problem into one of free fermions interacting with two fluctuating spin-1 Ising spin fields, each of size $N \times L$. The partition function becomes

$$\mathcal{Z} = \operatorname{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K] \prod_{i=0}^{N-1} \exp\left[-\Delta\tau \hat{V}_i\right] \right] \tag{3.28}$$

$$= \operatorname{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K] \prod_{i=0}^{N-1} \sum_{s_{il}, s'_{il}} \gamma_{s_{il}} \gamma_{s'_{il}} \exp\left[\lambda s_{il} (\hat{N}_i - 2) + \lambda' s'_{il} \hat{M}_i \right] \right] \tag{3.29}$$

$$= \operatorname{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K] \sum_{\mathbf{s}_l, \mathbf{s}'_l} \left(\prod_{i=0}^{N-1} \gamma_{s_{il}} \gamma_{s'_{il}} e^{-2\lambda s_{il}} \right) \exp\left[\sum_i \left(\lambda s_{il} \hat{N}_i + \lambda' s'_{il} \hat{M}_i \right) \right] \right] \tag{3.30}$$

$$= \sum_{\mathbf{s}\mathbf{s}'} \left(\prod_{il} \gamma_{s_{il}} \gamma_{s'_{il}} e^{-2\lambda s_{il}} \right) \operatorname{Tr}\left[\prod_{l=0}^{L-1} \exp[-\Delta\tau K] \exp\left[\sum_i \left(\lambda s_{il} \hat{N}_i + \lambda' s'_{il} \hat{M}_i \right) \right] \right] = \sum_{\mathbf{s}\mathbf{s}'} w(\mathbf{s}, \mathbf{s}') \tag{3.31}$$

where after applying Eq. (2.9),

$$w(\mathbf{s}, \mathbf{s}') = \left(\prod_{il} \gamma_{s_{il}} \gamma_{s'_{il}} e^{-2\lambda s_{il}} \right) \det\left(I + \prod_{l=0}^{L-1} \exp[-\Delta\tau \mathbf{k}] \exp\left[\sum_i \left(\lambda s_{il} \mathbf{N}_i + \lambda' s'_{il} \mathbf{M}_i \right) \right] \right)$$

$$= p_{\mathbf{ss}'} \det\left(I + B_{\mathbf{ss}'}\right), \quad (3.32)$$

where $\mathbf{k}, \mathbf{N}, \mathbf{M}$ are $4N \times 4N$ (N is total number of unit cells) matrices of numbers, corresponding to the kinetic matrix $\hat{H}_0$, density $\hat{N} = \sum_i \hat{N}_i$, and layer polarization $\hat{M} = \sum_i \hat{M}_i$ terms, respectively. The prefactor $p_{\mathbf{ss}'}$ is always positive. For this model, the correct anti-unitary operator to write down is (sorry for the notation, $\hat{K}$ has nothing to do with K and $\mathbf{k}$)

$$\hat{T} = \sum_{i\sigma} \left[|i, A, \sigma\rangle\langle i, B, \sigma| - |i, B, \sigma\rangle\langle i, A, \sigma|\right] \hat{K}, \quad (3.33)$$

where $\hat{K}$ is the complex conjugation operator. Then one shows that $\hat{T}\mathbf{k}\hat{T}^{-1} = \mathbf{k}$ always, but

$$\hat{T}\lambda\mathbf{N}\hat{T}^{-1} = \lambda^*\mathbf{N} \quad \hat{T}\lambda'\mathbf{M}\hat{T}^{-1} = -(\lambda')^*\mathbf{M} \quad (3.34)$$

when λ is purely real, and λ' is purely imaginary, which is true iff $|U| \leq V$. This establishes a parameter regime satisfying sufficient conditions for $w(\mathbf{s}, \mathbf{s}')$ to be positive semi-definite.

I didn't have time to talk about the other class (Majorana class) of sign-free models in these notes. If you'd like to learn more, hopefully [LJY16, LY19, HCH+20, GB23] and references therein are helpful.

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