A Solution to the Sign Problem Using a Sum-of-Few-Fermions Hamiltonian

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Abstract: A restricted path integral method is proposed to efficiently simulate a class of quantum systems and Hamiltonians called sum-of-few-fermions (SFF) by Monte Carlo on a classical computer without a numerical sign problem. Then a universality is proven to assert that any bounded-error quantum polynomial time (BQP) algorithm can be mapped to the ground state of an SFF Hamiltonian and becomes efficiently simulatable. Therefore, the computational complexity class of bounded-error probabilistic polynomial time (BPP) is precisely the same as the class of BQP.

The ability to simulate quantum systems efficiently on a programmable computer, classical [1,2] or quantum [1,3,4], is crucially important for fundamental sciences and practical applications. Of particular importance is to simulate the ground state of a many-body quantum system efficiently on a classical computer. Among many numerical methods, quantum Monte Carlo (QMC) [2] is uniquely advantageous as being based on first principles without uncontrolled systematic errors and using polynomially efficient importance sampling from an exponentially large Hilbert space, until its polynomial efficiency is spoiled by the notorious numerical sign problem [5,6]. On the other hand, a fundamental question in computational complexity theory is whether the complexity class of bounded-error probabilistic polynomial time (BPP) is the same as that of bounded-error quantum polynomial time (BQP) [7], which will be answered affirmatively in this presentation by firstly identifying and characterizing a class of Hamiltonians callws sum-of-few-fermions (SFF), whose Gibbs kernels and ground states are amenable to efficient Monte Carlo simulations on a classical computer, then demonstrating that a universal BQP algorithm can be mapped into an SFF Hamiltonian, therefore, QMC simulated efficiently [8].

Let a triple $(\mathcal{C},\mathcal{H},\mathcal{B})$ represent a general quantum system [8], where $\mathcal{C}$ is a *configuration space* consisting of eigenvalues of a collection of dynamical variables associated with the quantum system, for example but not limited to spatial positions of particles, while $\mathcal{H} \stackrel{\text{def}}{=} \mathcal{H}(\mathcal{C}) \subseteq L^2(\mathcal{C})$ is a Hilbert space of state vectors (*i.e.*, wavefunctions) supported by $\mathcal{C}$, and $\mathcal{B} \stackrel{\text{def}}{=} \mathcal{B}(\mathcal{H})$ is a Banach algebra of bounded operators acting on vectors in $\mathcal{H}$, which contains a strongly continuous one-parameter semigroup of Gibbs operators $\{\exp(-\tau H)\}_{\tau\in[0,\infty)}$, whose infinitesimal generator H is designated as the Hamiltonian for the quantum system. A Hamiltonian is the epitome of a general lower-bounded self-adjoint operator h, called a *partial Hamiltonian*, whose lowest eigenvalue is denoted by $\lambda_0(h)\in\mathbb{R}$, and the associated ground state is denoted by $\psi_0(h)$, as either a non-degenerate wavefunction or an arbitrary representative of the equivalence class of vectors in the ground state subspace. It is assumed that all fundamental equations of physics, especially the Schrödinger and quantum field-theoretic equations, are nondimensionalized and written in a so-called natural unit system. It is without loss of generality (WLOG) to assume that $\mathcal{C}$ is a compact Riemannian manifold with a finite dimension $\dim(\mathcal{C})\in\mathbb{N}$ and a finite diameter $\operatorname{diam}(\mathcal{C})\in\mathbb{R}$, thus a finite $\operatorname{size}(\mathcal{C}) \stackrel{\text{def}}{=} \dim(\mathcal{C})+\operatorname{diam}(\mathcal{C})$, and all wavefunctions are real-valued, so the Hilbert spaces and Banach algebras are over $\mathbb{R}$ [7–10].

Consider a *many-fermion system* (MFS) of a variable size, comprising a number $S\in\mathbb{N}$ of fermion species, each species labeled by $s\in[1,S]$ consisting of a number $n_s\in\mathbb{N}$ of identical fermions moving on a low-dimensional Riemannian manifold $\mathcal{X}_s$, where the total number of particles $N_* \stackrel{\text{def}}{=} \sum_{s=1}^{S} n_s$ may go up unbounded, while both $d_s \stackrel{\text{def}}{=} \dim(\mathcal{X}_s)$ and $D_s \stackrel{\text{def}}{=} \operatorname{diam}(\mathcal{X}_s)$, $\forall s\in[1,S]$ are always bounded by a finite number independent of N_*. Mathematically, the identical fermions of each species $s\in[1,S]$ may be artificially labeled by an integer $n\in[1,n_s]$, so that a configuration coordinate (point) $q_s \stackrel{\text{def}}{=} (q_{s1},q_{s2},\cdots,q_{sn_s})\in\mathcal{X}_s^{n_s}$ can represent their spatial configuration. But physically, the indistinguishability among identical fermions dictates that all of the label-exchanged coordinates be equivalent and form an orbit $\mathcal{G}_s q_s \stackrel{\text{def}}{=} \{\pi_s q_s : \pi_s\in\mathcal{G}_s\}$ for any $q_s\in\mathcal{X}_s^{n_s}$, where $\mathcal{G}_s$ is the symmetry group of permuting n_s labels, $\pi_s\in\mathcal{G}_s$ is a typical permutation. Straightforwardly, the Cartesian product $\mathcal{C} \stackrel{\text{def}}{=} \prod_{s=1}^{S}\mathcal{X}_s^{n_s}$ is a configuration space for the MFS, and the group direct product $G_* \stackrel{\text{def}}{=} \prod_{s=1}^{S}\mathcal{G}_s$, called the *exchange symmetry group* of the MFS, acts on $\mathcal{C}$ and partitions it into disjoint

orbits. Clearly, every pair of permutations $\pi \in \mathcal{G}_s$, $s \in [1,S]$ and $\pi' \in \mathcal{G}_{s'}$, $s' \in [1,S]$ with $s \neq s'$ commute, hence each $\mathcal{G}_s$, $s \in [1,S]$ is straightforwardly a normal subgroup of G_*. All of the even permutations in G_* form a subgroup A_*, called the *exchange alternating group*. It is an axiom of physics that any legitimate quantum state $\psi \in \mathcal{H}(\mathcal{C})$ must be exchange-symmetric as $[\pi\psi](q) \stackrel{\text{def}}{=} \psi(\pi q) = (-1)^\pi \psi(q)$, $\forall q \in \mathcal{C}$, $\forall \pi \in G_*$. With respect to G_* and its actions on $\mathcal{C}$ and $\mathcal{H}(\mathcal{C})$, an exchange symmetrization operator is defined as $\mathcal{P} \stackrel{\text{def}}{=} \sum_{\pi \in G_*} (-1)^\pi \pi$, up to a normalization constant.

For any partial Hamiltonian h, and any $(r,q,\tau) \in \mathcal{C}^2 \times (0,\infty)$, let $\langle r|e^{-\tau h}|q\rangle$ represent an artificial, non-negative definite, boltzmannonic Gibbs transition amplitude from q to r in (imaginary) time τ due to h, which ignores the fermionic exchange symmetry and regards all particles distinguishable, let $\langle r|e^{-\tau h}|\mathcal{P}q\rangle \stackrel{\text{def}}{=} \sum_{\pi \in G_*} (-1)^\pi \langle r|e^{-\tau h}|\pi q\rangle$ or $\langle \mathcal{P}r|e^{-\tau h}|q\rangle \stackrel{\text{def}}{=} \sum_{\pi \in G_*} (-1)^\pi \langle \pi r|e^{-\tau h}|q\rangle$ denote a pre- or post-symmetrized fermionic Gibbs transition amplitude. The function $\langle \cdot|e^{-\tau h}|\cdot\rangle \in L^2(\mathcal{C}^2)$ is called the boltzmannonic Gibbs kernel, and $\langle \cdot|e^{-\tau h}|\mathcal{P}\cdot\rangle \in L^2(\mathcal{C}^2)$ or $\langle \mathcal{P}\cdot|e^{-\tau h}|\cdot\rangle \in L^2(\mathcal{C}^2)$ is called the pre- or post-symmetrized fermionic Gibbs kernel, associated with a Gibbs operator $\exp(-\tau h)$, $\tau \in (0,\infty)$ generated by a partial Hamiltonian h. It is obvious that $\langle \cdot|e^{-\tau h}|\mathcal{P}\cdot\rangle \equiv \langle \mathcal{P}\cdot|e^{-\tau h}|\cdot\rangle$, either one may be referred to as the fermionic Gibbs kernel.

Given an MFS governed by a Hamiltonian H, a computationally important number is the (descriptive) size of H, denoted by $\text{size}(H)$, which is basically the minimum number of classical bits, up to a constant factor, that is needed to describe H. All computational complexities and singular values of operators will be measured against $\text{size}(H)$. Of great interests are the so-called (computationally) local Hamiltonians [11,12] of the form $H = \sum_{k=1}^K H_k$, $K \in \mathbb{N}$, $K = O(\text{poly}(N_*))$, where the size of H is defined as $\text{size}(H) \stackrel{\text{def}}{=} \text{size}(\mathcal{C}) + K$, thus $\text{size}(H) = O(\text{poly}(N_*))$, each H_k, $k \in [1,K]$ moves a small number of artificially labeled fermions. By an H_k, $k \in [1,K]$ moving an n-th fermion of an s-th species, $s \in [1,S]$, $n \in [1,n_s]$, it is meant that there exist a $\tau \in (0,\infty)$ and two configuration points $q = (\cdots q_{sn} \cdots) \in \mathcal{C}$ and $r = (\cdots r_{sn} \cdots) \in \mathcal{C}$, such that $r_{sn} \neq q_{sn}$ while the boltzmannonic Gibbs transition amplitude $\langle r|e^{-\tau H_k}|q\rangle \neq 0$ [8].

One exemplary local Hamiltonian describes an MFS having a single fermion species with a large number of identical particles, which is a conventional Schrödinger operator $H = \frac{1}{2}\sum_{n=1}^{N_*} \partial^2/\partial x_n^2 + V(x_1,\cdots,x_{N_*})$, but rewritten into a local Hamiltonian as $H = \sum_{n=1}^{N_*} H_n$, with each partial Hamiltonian moving three artificially labeled fermions as $H_n \stackrel{\text{def}}{=} \frac{1}{6}\sum_{k=n-1}^{n+1} \partial^2/\partial x_{k\parallel N_*} + V(x_1,\cdots,x_{N_*})/N_*$, $\forall n \in [1,N_*]$, where $k \parallel N_*$ denotes the unique number in $[1,N_*]$ such that $k - (k \parallel N_*) \equiv 0 \pmod{N_*}$, $\forall k \in \mathbb{N}$.

Another exemplary local Hamiltonian $H = \sum_{k=1}^K H_k$ describes an important class of MFS called a *many-species fermionic system (MSFS)*, that comprises a large number $S \in \mathbb{N}$ of fermion species, each of which has no more than a small constant of identical fermions, where each H_k, $k \in [1,K]$ moves either all or none of the identical particles of any fermion species. For each $k \in [1,K]$, the species and fermions moved by H_k constitute a subsystem called a *few-fermion cluster*, or just a *few-fermion* in short, which is associated with a factor subspace $\mathcal{C}_k$ and a factor subgroup $G_k \leq G_*$, in the sense that, $\mathcal{C}'_k$ and $G'_k \leq G_*$ exist such that $\mathcal{C}_k \times \mathcal{C}'_k \simeq \mathcal{C}$ and $G_k \times G'_k \simeq G_*$. Obviously, each G_k, $k \in [1,K]$ is a normal subgroup of G_* and itself a direct product of a small number of normal subgroups from the list $\{\mathcal{G}_s\}_{s\in[1,S]}$.

Definition 1. *Given an MSFS with a variable number $S \in \mathbb{N}$ of fermion species, a form sum $H = \sum_{k=1}^K H_k$, $K = O(\text{poly}(S))$ defining a local Hamiltonian is called a sum of few-fermions, when each H_k, $k \in [1,K]$, called a few-fermion interaction (FFI), involves no more than a small constant number of fermion species, moves either all or none of the identical particles of each involved fermion species, and is invariant under any exchange of identical particles, namely, $\pi^{-1} H_k \pi = H_k$, $\forall \pi \in \mathcal{G}_*$.*

Such MSFS and H are said to be sum-of-few-fermions (SFF), with sum-of-few-fermions (SFF) serving as an adjective. Although an SFF system may have a large total number of particles N_*, each FFI H_k, $k \in [1,K]$ corresponds to a few-fermion comprising a small number of fermions and species. Due to the small size of a few-fermion, it is always computationally easy, with the complexity bounded by a constant, to solve any H_k, $k \in [1,\mathsf{k}]$ or any associated Gibbs kernel or any related physics, either analytically or numerically.

Definition 2. *Let $H = \sum_{k=1}^K H_k$ be a form sum defining an SFF Hamiltonian. The form sum is called a Lie-Trotter-Kato (LTK) decomposition, and H is called LTK-decomposed, when $\forall \epsilon > 0$, there exists an $m \in \mathbb{N}$, $m = O(\text{poly}(\text{size}(H) + \epsilon^{-1}))$, such that $\langle r|\{\prod_{k=1}^K e^{-H_k/m}\}^m|\mathcal{P}q\rangle \in \langle r|e^{-H}|\mathcal{P}q\rangle\,(1-\epsilon, 1+\epsilon)$, $\forall (r,q) \in \mathcal{C}^2$*

satisfying $|\langle r|e^{-H}|\mathcal{P}q\rangle| > \epsilon\, e^{-\lambda_0(H)}$. *The same form sum is called a ground-state projection (GSP) decomposition, and* H *is called GSP-decomposed, when* $\forall \epsilon > 0$, *there exists an* $m \in \mathbb{N}$, $m = O(\mathrm{poly}(\mathrm{size}(H) + \epsilon^{-1}))$, *such that* $\|\{\prod_{k=1}^{K} \Pi_k\}^m - \Pi_*\| < \epsilon$, *where* $\|\cdot\|$ *denotes the operator norm,* $\Pi_* \stackrel{\text{def}}{=} \lim_{\tau\to\infty} e^{-\tau[H-\lambda_0(H)]}$ *and* $\Pi_k \stackrel{\text{def}}{=} \lim_{\tau\to\infty} e^{-\tau[H_k-\lambda_0(H_k)]}$ *are projections to the ground state subspaces of* H *and* H_k, $k \in [1, K]$.

The definition of an LTK- or GSP-decomposed Hamiltonian is inspired by the LTK product formula $e^{-\tau H} = \lim_{m\to\infty}\{\prod_{k=1}^{K} e^{-\tau H_k/m}\}^m$, $\tau \in (0,\infty)$, which suggests to divide $[0,\tau]$ into time intervals delimited by time instants $\{\tau_n \stackrel{\text{def}}{=} (n/K)\,\delta\tau\}_{n\in[0,N]}$, $\delta\tau \stackrel{\text{def}}{=} \tau/m$, $N \stackrel{\text{def}}{=} mK$, and break the Gibbs operator $e^{-\tau H}$ down into a sequence of Gibbs operators $\{\mathsf{G}_n \stackrel{\text{def}}{=} e^{-\delta\tau H_{n\|K}}\}_{n\in[1,N]}$, so to compute Gibbs kernels using the Feynman path integral, also known as the functional integration [13,14]. $n \,\|\, K$ denotes the unique number in $[1, K]$ such that $n-(n \,\|\, K) \equiv 0 \pmod K$, $\forall n \in \mathbb{N}$. Each Gibbs operator G_n and the spacetime domain $\mathcal{C}\times[\tau_{n-1},\tau_n]$, $n \in [1, N]$ constitute a *Feynman slab*, delimited by two *Feynman planes* $(\mathcal{C}_{n-1},\tau_{n-1}) \stackrel{\text{def}}{=} \{(q_{n-1},\tau_{n-1}) : q_{n-1} \in \mathcal{C}\}$ and $(\mathcal{C}_n,\tau_n) \stackrel{\text{def}}{=} \{(q_n,\tau_n) : q_n \in \mathcal{C}\}$ [8]. If necessary, each Feynman slab associated with a constant FFI $H_{n\|K}$, $n \in [1, N]$ can be further divided into thinner *Feynman slices* so that the Gibbs operators are easier to compute or approximate.

A number of consecutive Feynman slabs with the corresponding sequence of Gibbs operators $\{\mathsf{G}_n\}_{n\in[n_1,n_2]}$, $0 < n_1 \le n_2 \le N$ constitute a *Feynman stack* with the two Feynman planes $(\mathcal{C}_{n_1-1},\tau_{n_1-1})$ and $(\mathcal{C}_{n_2},\tau_{n_2})$ forming its boundaries [8]. Let $n_0 \stackrel{\text{def}}{=} n_1 - 1$, $\forall n_1 \in \mathbb{N}$. Pick two points $q_{n_0} \in \mathcal{C}_{n_0}$ and $q_{n_2} \in \mathcal{C}_{n_2}$ on the two boundary Feynman planes, the set of all Feynman paths

$$\Gamma(q_{n_2},\tau_{n_2};q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \{\gamma(t) : t \in [\tau_{n_0},\tau_{n_2}] \mapsto \mathcal{C} \text{ such that } \gamma(\tau_{n_0}) = q_{n_0},\, \gamma(\tau_{n_2}) = q_{n_2}\} \tag{1}$$

together with the sequence of partial Hamiltonians $\{H_{n\|K}\}_{n\in[n_1,n_2]}$ constitute a *Feynman spindle* [8], which gives rise to two Gibbs transition amplitudes, one being boltzmannonic and defined as

$$\rho(q_{n_2},\tau_{n_2};q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \int\cdots\int \Big\{\prod_{n=n_1}^{n_2} \langle q_n|e^{-\delta\tau H_{n\|K}}|q_{n-1}\rangle\Big\}\Big\{\prod_{n=n_1}^{n_2-1} dq_n\Big\}, \tag{2}$$

the other being fermionic and symmetrized as

$$\rho(q_{n_2},\tau_{n_2};\mathcal{P}q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \sum\nolimits_{\pi\in G_*} (-1)^\pi \rho(q_{n_2},\tau_{n_2};\pi q_{n_0},\tau_{n_0})\,. \tag{3}$$

In equation (2), the fermionic exchange symmetry is ignored and the integration over all particle-distinguished Feynman paths yields a non-negative definite, boltzmannonic Gibbs transition amplitude. On the right side of equation (3), even though the whole group G_* is used for the domain of exchange symmetry, it is really only those permutations in the subgroup $G_{n_1:n_2}$ generated by the set of subgroups $\{G_n = G_{n\|K}\}_{n=n_1}^{n_2}$ that are active and relevant, since $\rho(q_{n_2},\tau_{n_2};\pi q_{n_0},\tau_{n_0}) = 0$ for all $\pi \notin G_{n_1:n_2}$.

For Feynman slabs or slices that are sufficiently thin, there are simple rules for *Feynman flights* [8], which determine the associated Gibbs transition amplitude between two points q and r on two narrowly separated Feynman planes respectively [13,14]. It is almost always the case, here taken as an axiomatic premise, that all partial Hamiltonians in consideration are of the Schrödinger type, as a sum of an elliptic differential operator $-\Delta$ and a bounded potential V, so to substantiate the *Hopf lemma* and the *strong Hopf extremum principle* [8, 15, 16], and ensure that the boltzmannonic Gibbs transition amplitude of a Feynman flight becomes exponentially localized as $\langle r|e^{-\delta\tau(-\Delta+V)}|q\rangle \le c_1 e^{-c_2\,\mathrm{dist}(r,q)^2/\delta\tau^{c_3}}$ when $\delta\tau > 0$ approaches 0, where c_1, c_2, c_3 are positive constants, $\mathrm{dist}(r,q)$ denotes the geodesic distance between q and r on the Riemannian manifold $\mathcal{C}$. Said rules for Feynman flights induce a Wiener measure that assigns a non-negative amplitude $W(\gamma) = e^{-U(\gamma)}$ to each Feynman path γ. Importantly, the action functional $U(\gamma)$ is linear with respect to path concatenation, in that $U(\gamma) = U(\gamma_1) + U(\gamma_2)$ holds when two segments of Feynman paths γ_1 and γ_2 concatenate into a continuous Feynman path $\gamma \stackrel{\text{def}}{=} \gamma_2 * \gamma_1$, which starts at the start point of γ_1, goes to the end point of γ_1 that coincides with the start point of γ_2, and continues till the end point of γ_2.

The formulation of Feynman path integral is rightly suited for simulating a Gibbs kernel via Monte Carlo integration over a many- but finite-dimensional space. Path integral Monte Carlo would realize BPP simulations of quantum systems, were it not for the sign problem [5,6] due to the presence of negative amplitudes, particularly in fermionic systems. QMC methods using *restricted path integrals* (RPIs) [6, 17–20] have been proposed and applied to avoid negative amplitudes. But previous RPIs are only approximate methods as

they rely on *a priori* approximations for the nodal surfaces of Gibbs kernels associated with the total Hamiltonian, which are unknown and hard to compute. Here I will show that for an SFF Hamiltonian, negative amplitudes can be avoided by restricting Feynman paths locally, with respect to the efficiently computable nodal surface of a Gibbs kernel associated with an individual FFI.

By Feynman's rule of amplitude multiplication for events occurring in succession [13], also known as the Chapman-Kolmogorov equation in probability theory, in conjunction with the (anti)symmetry of Gibbs kernels under particle exchanges, the fermionic Gibbs transition amplitude due to a Feynman stack, from a start point $q_{n_0} \in \mathcal{C}_{n_0}$ at τ_{n_0}, $n_0 = n_1 - 1$ to an end point $q_{n_2} \in \mathcal{C}_{n_2}$ at τ_{n_2}, can be computed as

$$\begin{aligned}
\rho(q_{n_2},\tau_{n_2};\mathcal{P}q_{n_0},\tau_{n_0}) &= \int_{q_{n_1}\in\mathcal{C}_{n_1}} \rho(q_{n_2},\tau_{n_2};q_{n_1},\tau_{n_1})\,\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1} \\
&= \int_{q_{n_1}\in\mathcal{R}_{n_1}} \rho(q_{n_2},\tau_{n_2};q_{n_1},\tau_{n_1})\,\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1} \\
&\propto \int_{q_{n_1}\in\mathcal{R}_{n_1}/G_*} \sum\nolimits_{\pi\in G_*} \rho(q_{n_2},\tau_{n_2};\pi q_{n_1},\tau_{n_1})\,\rho(\pi q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1} \qquad (4)\\
&\propto \int_{q_{n_1}\in\mathcal{R}_{n_1}/G_*} \sum\nolimits_{\pi\in G_*} \rho(q_{n_2},\tau_{n_2};\pi q_{n_1},\tau_{n_1})\,(-1)^{\pi}\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1} \\
&\propto \int_{q_{n_1}\in\mathcal{R}_{n_1}/G_*} \rho(q_{n_2},\tau_{n_2};\mathcal{P}q_{n_1},\tau_{n_1})\,\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1},
\end{aligned}$$

where $\mathcal{R}_{n_1} \stackrel{\text{def}}{=} \mathcal{R}_{n_1}(q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \{q_{n_1}\in\mathcal{C}_{n_1} : \rho(q_{n_1},\tau_{n_1};q_{n_0},\tau_{n_0}) > 0\} \subseteq \mathcal{C}_{n_1}$ is called the *boltzmannonic range* of q_{n_0} from τ_{n_0} to τ_{n_1}, "$\propto$" indicates an equality up to a universal (that is, $(q_{n_2},q_{n_1},q_{n_0})$-independent) constant, $\mathcal{R}_{n_1}/G_*$ is any subset of $\mathcal{R}_{n_1}$ that tiles up $\mathcal{R}_{n_1}$ under the action of G_*, *i.e.*, $\bigcup_{\pi\in G_*}\pi(\mathcal{R}_{n_1}/G_*) \supseteq \mathcal{R}_{n_1}$. It suffices to choose $\mathcal{R}_{n_1}/G_* = \mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \big\{q_{n_1}\in\mathcal{R}_{n_1} : \rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0}) > 0\big\}$, which is the set union of all of the positive nodal cells of $\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})$ regarded as a function of $q_{n_1}\in\mathcal{C}_{n_1}$, having q_{n_0}, τ_{n_0}, τ_{n_1} fixed. Similarly, let $\mathcal{N}^-_{n_1}(q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \big\{q_{n_1}\in\mathcal{R}_{n_1} : \rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0}) < 0\big\}$ denote the set union of all of the negative nodal cells. Clearly, any odd permutation $\pi\in G_*\backslash A_*$ induces a one-to-one correspondence between the set of positive nodal cells and the set of negative nodal cells. Therefore,

$$\rho(q_{n_2},\tau_{n_2};\mathcal{P}q_{n_0},\tau_{n_0}) \propto \int_{q_{n_1}\in\mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0})} \rho(q_{n_2},\tau_{n_2};\mathcal{P}q_{n_1},\tau_{n_1})\,\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})\,dq_{n_1}. \qquad (5)$$

In general, it has been rigorously proved that, under the action of the group G_*, any nodal cell $\mathcal{N}_{n_1}$ tiles up the configuration subspace $\mathcal{R}_{n_1}$, thus, $\mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0}) = A_*\mathcal{N}_{n_1}(q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \bigcup_{\pi\in A_*}\pi\mathcal{N}_{n_1}(q_{n_0},\tau_{n_0})$, provided that the FFIs are of the Schrödinger type and substantiate the Hopf lemma and the strong Hopf extremum principle [6, 8]. Moreover, any wavefunction or Gibbs kernel over $\mathcal{R}_{n_1}$ is fully determined by and easily recovered from its restriction on $\mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0})$.

Now consider $\rho(q,\tau;\mathcal{P}q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \langle q|e^{-(\tau-\tau_{n_0})KH_{n_1\|K}}|\mathcal{P}q_{n_0}\rangle$ as a (q,τ)-jointly continuous function of $(q,\tau)\in\mathcal{C}\times(\tau_{n_0},\tau_{n_1}+\delta_1)$, $\delta_1 > 0$. The preimage $\{(q,\tau) : \rho(q,\tau;\mathcal{P}q_{n_0},\tau_{n_0}) > 0\}$ is an open set, the connected component of which containing the trivial node-free path $\{(q_{n_0},\tau) : \tau\in(\tau_{n_0},\tau_{n_1}]\}$ is called the *nodal tube* or the *Ceperley reach* of $q_{n_0}\in\mathcal{C}_{n_0}$ [6,8], which is denoted by $\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$. Let $\mathcal{T}_{n_1}(\tau;q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})\cap\mathcal{C}\times\{\tau\}$, $\forall\tau\in(\tau_{n_0},\tau_{n_1}]$, which is clearly a nodal cell of the fermionic Gibbs kernel $\rho(q,\tau;\mathcal{P}q_{n_0},\tau_{n_0})$ as a function of $q\in\mathcal{C}$. It is well known that, inside the nodal tube $\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$, the fermionic Gibbs kernel $\rho(q,\tau;\mathcal{P}q_{n_0},\tau_{n_0})$ coincides with an RPI $\rho_R(q,\tau;q_{n_0},\tau_{n_0})$, which is a boltzmannonic path integral over all particle-distinguished Feynman paths that lie fully within the nodal tube $\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$ [6,8,17–20].

In a hypothetical procedure of numerical integration, the fermionic Gibbs kernel $\rho(q_{n_1},\tau_{n_1};\mathcal{P}q_{n_0},\tau_{n_0})$ as a function of $q_{n_1}\in\mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0})$ may be sampled using two nested loops, where an outer loop moves the configuration coordinate $q_{n_1}\in\mathcal{N}^+_{n_1}(q_{n_0},\tau_{n_0})$, while an inner loop regards q_{n_0} and q_{n_1} being fixed, samples from the set $\Gamma(q_{n_1},\tau_{n_1};G_*q_{n_0},\tau_0) \stackrel{\text{def}}{=} \bigcup_{\pi\in G_*}\Gamma(q_{n_1},\tau_{n_1};\pi q_{n_0},\tau_0)$ of Feynman paths that connect a start point in the orbit $G_*q_{n_0}$ to the end point q_{n_1}, and integrates the signed Wiener measure $(-1)^{\pi}W(\gamma)$ for each Feynman path γ connecting a certain πq_{n_0}, $\pi\in G_*$ to q_{n_1}. It turns out that any Feynman path crossing or making contact with the boundary of the nodal tubes $\{\partial\mathcal{T}_{n_1}(\pi q_{n_0},\tau_{n_0})\}_{\pi\in A_*}$ belongs to a G_*-orbit of sets of Feynman paths that integrate to a net zero amplitude, so all of which can be removed from path integration. Specifically, let γ_1 denote a segment of Feynman path connecting a point $(q,\tau)\in\partial\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$,

$\tau \in (\tau_{n_0}, \tau_{n_1}]$ to the end point q_{n_1}, then for each $\pi \in G_*$, the set of concatenated Feynman paths

$$\gamma_1 * \Gamma(q,\tau;\pi q_{n_0},\tau_{n_0}) \stackrel{\text{def}}{=} \{\gamma_1 * \gamma_0 : \gamma_0 \in \Gamma(q,\tau;\pi q_{n_0},\tau_{n_0})\},$$

together with the relevant FFIs constitute a *post-tethered Feynman spindle*, which yields a Wiener measure $\int_{\gamma_0 \in \Gamma(q,\tau;\pi q_{n_0},\tau_{n_0})} W(\gamma_1)\, W(\gamma_0)\, d\gamma_0 = W(\gamma_1)\, \rho(q,\tau;\pi q_{n_0},\tau_{n_0})$. With π traversing the group G_*, it enumerates a G_*-orbit of post-tethered Feynman spindles associated with $\{\gamma_1 * \Gamma(q,\tau;\pi q_{n_0},\tau_{n_0})\}_{\pi \in G_*}$, whose corresponding Wiener measures should be signed accordingly and summed up to yield

$$\sum\nolimits_{\pi \in G_*} W(\gamma_1)\, (-1)^{\pi} \rho(q,\tau;\pi q_{n_0},\tau_{n_0}) \;=\; W(\gamma_1)\, \rho(q,\tau;\mathcal{P} q_{n_0},\tau_{n_0}) \;=\; W(\gamma_1)\, \rho(\mathcal{P} q,\tau;q_{n_0},\tau_{n_0}), \qquad (6)$$

which makes a net zero contribution to $\rho(q_{n_1},\tau_{n_1};\mathcal{P} q_{n_0},\tau_{n_0})$, when $(q,\tau) \in \partial\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$. Moreover, it is obvious that the same analysis applies to a more general G_*-orbit of post-tethered Feynman spindles associated with $\{\gamma_1' * \Gamma(q,\tau;\pi q_{n_0},\tau_{n_0})\}_{\pi \in G_*}$, where $\tau \in (\tau_{n_0},\tau_{n_1}]$, and γ_1' is a Feynman path connecting the point (q,τ) to any point $(q',\tau') \in \mathcal{C} \times (\tau_{n_1},\tau_N]$, including $(q',\tau') = (q_N,\tau_N)$, so to conclude that any Feynman path crossing or making contact with the boundary of the nodal tube $\partial\mathcal{T}_{n_1}(q_{n_0},\tau_{n_0})$ belongs to a G_*-orbit of sets of Feynman paths that make a net zero contribution to the Gibbs transition amplitude $\rho(q',\tau';\mathcal{P} q_{n_0},\tau_{n_0})$, thus can be safely removed from path integration. The only thing to note is that the calculation of the Wiener measure $W(\gamma_1')$ for the path γ_1' may involve other FFIs than H_{n_1}.

Still further, it is straightforward to write the fermionic Gibbs kernel in the post-symmetrized from as $\rho(\mathcal{P} q_{n_1},\tau_{n_1};q_{n_0},\tau_{n_0})$ and apply exactly the same analyses on a G_*-orbit of *pre-tethered Feynman spindles* associated with

$$\big\{\Gamma(\pi q_{n_1},\tau_{n_1};q,\tau) * \gamma_0 \stackrel{\text{def}}{=} \{\gamma_1 * \gamma_0 : \gamma_1 \in \Gamma(\pi q_{n_1},\tau_{n_1};q,\tau)\}\big\}_{\pi \in G_*},$$

where γ_0 is a segment of Feynman path connecting (q_{n_0},τ_{n_0}) to $(q,\tau) \in \mathcal{T}^*_{n_1}(q_{n_1},\tau_{n_1})$, $\Gamma(\pi q_{n_1},\tau_{n_1};q,\tau)$ is the set of Feynman paths associated with the Feynman spindle between (q,τ) and $(\pi q_{n_1},\tau_{n_1})$ for each $\pi \in G_*$, and $\mathcal{T}^*_{n_1}(q_{n_1},\tau_{n_1})$ is a *backward nodal tube* for the Gibbs kernel $\rho(\mathcal{P} q_{n_1},\tau_{n_1};q',\tau') \stackrel{\text{def}}{=} \langle \mathcal{P} q_{n_1}| e^{-(\tau_{n_1}-\tau')K H_{n_1 \| K}} |\rho'\rangle$ regarded as a function of $(\rho',\tau') \in \mathcal{C} \times (\tau_{n_0}-\delta_0,\tau_{n_1})$, $\delta_0 > 0$ with respect to the fixed $q_{n_1} \in \mathcal{C}_{n_1}$ and τ_{n_1}, where $\mathcal{T}^*_{n_1}(q_{n_1},\tau_{n_1})$ is the connected component of the open set $\{(q',\tau') : \rho(\mathcal{P} q_{n_1},\tau_{n_1};q',\tau') > 0\}$ that contains the path $\{(q_{n_1},\tau') : \tau' \in [\tau_{n_0},\tau_{n_1})\}$. It is clear that any Feynman path crossing or touching the boundary of a backward nodal tube can be safely removed from path integration, and similarly, the purge of nodal surface-touching Feynman paths can be extended to when γ_0 starts at a time earlier than τ_{n_0}.

Consider a practical Markov chain Monte Carlo (MCMC) procedure that samples a dual-symmetrized Gibbs kernel $\rho(\mathcal{P} q_N,\tau_N;\mathcal{P} q_0,\tau_0)$ for the whole Feynman stack associated with the Gibbs operators $\{\mathsf{G}_n\}_{n \in [1,N]}$, where $(q_N,q_0) \in (\mathcal{C}/G_*)^2$, $\mathcal{C}/G_*$ can be any subset that tiles up $\mathcal{C}$ under the action of G_*. It follows from the above analyses and method of RPI that

$$\begin{aligned}
&\rho(\mathcal{P} q_N,\tau_N;\mathcal{P} q_0,\tau_0) \\
=\;& \int_{q_{N-1} \in \mathcal{C}_{N-1}} \int_{q_1 \in \mathcal{C}_1} \rho(\mathcal{P} q_N,\tau_N;q_{N-1},\tau_{N-1})\, \rho(q_{N-1},\tau_{N-1};q_1,\tau_1)\, \rho(q_1,\tau_1;\mathcal{P} q_0,\tau_0)\, dq_1 dq_{N-1} \\
\propto\;& \int_{q_{N-1} \in \mathcal{N}^+_N(q_N,\tau_N)} \int_{q_1 \in \mathcal{N}^+_1(q_0,\tau_0)} \sum\nolimits_{(\pi_{N-1},\pi_1) \in G_*^2} \rho(\mathcal{P} q_N,\tau_N;\pi_{N-1} q_{N-1},\tau_{N-1}) \\
\times\;& \rho(\pi_{N-1} q_{N-1},\tau_{N-1};\pi_1 q_1,\tau_1)\, \rho(\pi_1 q_1,\tau_1;\mathcal{P} q_0,\tau_0)\, dq_1 dq_{N-1} \qquad (7) \\
\propto\;& \int_{q_{N-1} \in \mathcal{N}^+_N(q_N,\tau_N)} \int_{q_1 \in \mathcal{N}^+_1(q_0,\tau_0)} \rho(\mathcal{P} q_N,\tau_N;q_{N-1},\tau_{N-1}) \\
\times\;& \rho(\mathcal{P} q_{N-1},\tau_{N-1};\mathcal{P} q_1,\tau_1)\, \rho(q_1,\tau_1;\mathcal{P} q_0,\tau_0)\, dq_1 dq_{N-1} \\
\propto\;& \int_{q_{N-1} \in \mathcal{N}_{N-1}(q_N,\tau_N)} \sum\nolimits_{\pi_{N-1} \in A_*} \int_{q_1 \in \mathcal{N}_1(q_0,\tau_0)} \sum\nolimits_{\pi_1 \in A_*} \rho_R(\pi_{N-1} q_N,\tau_N;\pi_{N-1} q_{N-1},\tau_{N-1}) \\
\times\;& \rho(\mathcal{P} q_{N-1},\tau_{N-1};\mathcal{P} q_1,\tau_1)\, \rho_R(\pi_1 q_1,\tau_1;\pi_1 q_0,\tau_0)\, dq_1 dq_{N-1}\,,\; \forall (q_N,q_0) \in (\mathcal{C}/G_*)^2,
\end{aligned}$$

where $\mathcal{N}_1(q_0,\tau_0)$ is the nodal cell of $\rho(\cdot,\tau_1;\mathcal{P} q_0,\tau_0)$ at τ_1 enclosing q_0, and $\mathcal{N}_N(q_N,\tau_N) \stackrel{\text{def}}{=} \mathcal{T}_N(q_N,\tau_N) \cap (\mathcal{C} \times \{\tau_{N-1}\})$ is the *backward nodal cell* of $\rho(\mathcal{P} q_N,\tau_N;q_{N-1},\tau_{N-1})$ at τ_{N-1} enclosing q_N, $\mathcal{N}^+_1(q_0,\tau_0)$ and $\mathcal{N}^+_N(q_N,\tau_N)$ are the corresponding set unions of nodal cells and backward nodal cells respectively, while $\rho_R(\pi q_1,\tau_1;\pi q_0,\tau_0)$

and $\rho_R(\pi q_N, \tau_N; \pi q_{N-1}, \tau_{N-1})$ for any $\pi \in A_*$ are non-negative definite transition amplitudes computed using RPIs within the first and the last Feynman slabs respectively. In other words, the first and the last Feynman slabs have been *path rectified*, with the fermionic exchange and sign considerations no longer necessary and relevant. The same method of RPI can be repeated to have all Feynman slabs path rectified, such that

$$\begin{aligned}\rho(\mathcal{P}q_N, \tau_N; \mathcal{P}q_0, \tau_0) \propto & \left\{ \int_{q_n \in \mathcal{N}_n} \sum\nolimits_{\pi_n \in A_*} \right\}_{n=1}^{N-1} \rho_R(\pi_{N-1} q_N, \tau_N; \pi_{N-1} q_{N-1}, \tau_{N-1}) \\ & \times \prod\nolimits_{n=1}^{N-1} \rho_R(\pi_n q_n, \tau_n; \pi_n q_{n-1}, \tau_{n-1}) \prod\nolimits_{n=1}^{N-1} dq_n \,, \end{aligned} \tag{8}$$

$\forall (q_N, q_0) \in (\mathcal{C}/G_*)^2$, where $\mathcal{N}_n \stackrel{\text{def}}{=} \mathcal{N}_n(q_{n-1}, \tau_{n-1})$ for each $n \in [1, \lfloor N/2 \rfloor]$, $\lfloor N/2 \rfloor \stackrel{\text{def}}{=} \max\{n \in \mathbb{N} : 2n \le N\}$ represents the nodal cell of the pre-symmetrized Gibbs kernel of the n-th Feynman slab with respect to (q_{n-1}, τ_{n-1}), and $\mathcal{N}_n \stackrel{\text{def}}{=} \mathcal{N}^*_{n+1}(q_{n+1}, \tau_{n+1})$ for each $n \in [1 + \lfloor N/2 \rfloor, N-1]$ denotes the backward nodal cell of the post-symmetrized Gibbs kernel of the $(n+1)$-th Feynman slab with respect to (q_{n+1}, τ_{n+1}). Due to the frequent insertion of $\pi \in A_*$ permutations, the Feynman paths in a path integral such as equation (8) appear to undergo abrupt coordinate jumps in the space $\mathcal{C} \times (\tau_0, \tau_N]$, which do not represent actual physical discontinuities, since all points in any orbit $A_* q$, $q \in \mathcal{C}$ are physically equivalent and represent the same physical reality. Indeed, such Feynman paths are actually continuous in the space $(\mathcal{C}/A_*) \times (\tau_0, \tau_N]$, where $\mathcal{C}/A_*$ is an orbifold regarding each orbit $A_* q$, $q \in \mathcal{C}$ as a single point. A practical and effective means to incorporate such exchange equivalence is to associate each point (q_n, τ_n), $n \in [0, N]$ on a Feynman plane with two equivalent coordinates $q_n^- \in A_* q_n$ and $q_n^+ \in A_* q_n$, where q_n^- serves the Feynman stack or slice from τ_{n-1} to τ_n, and q_n^+ is used by the Feynman stack or slice from τ_n to τ_{n+1}.

It is worth noting that all path rectifications are done on a per Feynman slab basis, requires a solution for the nodal surface of the specific FFI associated with each Feynman slab, which can be obtained at no more than a constant computational cost due to the bounded number of fermion species moved by each FFI, while each species has a bounded number of identical particles. It is also important to note that the order in which the Feynman slabs are path rectified in equations (7) and (8) apparently creates a sequence of conditional dependence among the nodal cells on the Feynman planes and integrations over the corresponding configuration coordinates. However, such conditional dependence is insubstantial, since the order of the Feynman slabs being path rectified can be arbitrary, and different choices of such an order yields the same result for $\rho(\mathcal{P}q_N, \tau_N; \mathcal{P}q_0, \tau_0)$. Specifically, for any $n \in [1, N-1]$, if desired, the method of RPI can be applied iteratively such that the first to the $(n-1)$-th Feynman slabs are firstly path rectified in sequence, then the $(N-1)$-th to the $(n+1)$-th Feynman slabs are path rectified backward in order, leaving $\rho(\mathcal{P}q_{n-1}, \tau_{n-1}; \mathcal{P}q_{n+1}, \tau_{n+1})$ as the only fermionic and signed factor in the LTK product of Gibbs kernels, which is finally path rectified by discarding any Feynman path from a given $q_{n-1}^+ \in A_* q_{n-1}$ at τ_{n-1} to a given $q_{n+1}^- \in A_* q_{n+1}$ at τ_{n+1} that ever crosses or touches a nodal surface of either $\rho(q, \tau; \mathcal{P}q_{n-1}, \tau_{n-1})$, $\tau \in (\tau_{n-1}, \tau_n]$ or $\rho(\mathcal{P}q_{n+1}, \tau_{n+1}; q, \tau)$, $\tau \in [\tau_n, \tau_{n+1})$ as a function of $q \in \mathcal{C}$, $\forall \tau \in (\tau_{n-1}, \tau_{n+1})$. In particular, the fully rectified path integral integrates over the points q_n such that, both $q_n^- \in A_* q_n$ is in the Ceperley reach of q_{n-1}^+ with respect to $\langle \cdot | e^{-\delta\tau H_{n \| K}} | \mathcal{P} q_{n-1}^+ \rangle$, and $q_n^+ \in A_* q_n$ is in the Ceperley reach of q_{n+1}^- backward with respect to $\langle \mathcal{P} q_{n+1}^- | e^{-\delta\tau H_{(n+1) \| K}} | \cdot \rangle$. This perspective justifies a Monte Carlo subroutine that wiggles a Feynman path by walking only one coordinate on a single Feynman plane at any given time, subject to the constraint of no nodal crossing or touching in the two bordering Feynman slabs or slices.

In one exemplary embodiment of numerical simulation, a random and warm start $q_0 \in \mathcal{C}$ is chosen, and the RPI of equation (8) is approximated by running an MCMC procedure that starts with an initial Feynman path having $q_n = q_0$, $\forall n \in [0, N]$, and repeats two nested loops for a polynomial number of times, where an outer loop walks each coordinate q_{iK}, $i \in [0, m]$ in turn using a Metropolis-Hastings algorithm [21, 22] or Gibbs sampling [23] based on a conditional probability $\Pr(q_{iK} | \, q_{(i+1)K}^-, q_{(i-1)K}^+)$, with the index $i-1$ or $i+1$ being void and the coordinate $q_{(i-1)K}^+$ or $q_{(i+1)K}^-$ being omitted when $i = 0$ or $i = m$, while an inner loop samples from all of the restricted Feynman paths running from a fixed $q_{(i-1)K}^+ \in \mathcal{N}_{(i-1)K}^+$, passing a proposed $q_{iK}^- \sim q_{iK}^+ \sim q_{iK} \in \mathcal{N}_{iK}^+$, and finally reaching a fixed $q_{(i+1)K}^- \in \mathcal{N}_{(i+1)K}^+$, $\forall i \in [0, m]$, so to compute an RPI approximating the probability

$$\Pr(q_{iK} | \, q_{(i+1)K}^-, q_{(i-1)K}^+) \propto \rho_R(q_{(i+1)K}^-, \tau_{(i+1)K}; q_{iK}^+, \tau_{iK}) \, \rho_R(q_{iK}^-, \tau_{iK}; q_{(i-1)K}^+, \tau_{(i-1)K}) \,, \tag{9}$$

which coincides with the dual-symmetrized Gibbs kernel $\langle \mathcal{P} q_{(i+1)K} | e^{-\delta\tau H} | q_{iK} \rangle \langle q_{iK} | e^{-\delta\tau H} | \mathcal{P} q_{(i-1)K} \rangle$ as a func-

tion of $q_{iK} \in \mathcal{C}_{iK}/A_*$ restricted to a positive nodal cell. At each instant of time during either the inner or the outer loop, a random permutation $\pi \in A_*$ and two random integers $(n_1, n_2) \in [0, N]^2$, $n_1 < n_2$ can be chosen, such that a segment $\gamma(n_1 : n_2)$ of the instantaneous Feynman path that starts at τ_{n_1} and ends at τ_{n_2} can be transformed into $\pi\gamma(n_1 : n_2)$, where in particular, the sequence of points $\{(q_n, \tau_n) : n \in [n_1, n_2]\}$ as an element of the so-called cylinder set is transformed into $\{(\pi q_n, \tau_n) : n \in [n_1, n_2]\}$. The two nested loops create and operate at two timescales, where the inner loop is related to a short timescale, within which a random walk among the restricted Feynman paths mixes rapidly to yield a good estimate for $\Pr(q_{iK} | \, q^-_{(i+1)K}, q^+_{(i-1)K})$, while the outer loop is associated with a long timescale, in which the coordinates $\{q_{iK}\}_{i\in[0,m]}$ walk randomly and mix at a slower but still polynomial rate. The slow dynamics of the outer loop always sees the fast dynamics of the inner loop in its equilibrium at any instant on the long timescale.

Specifically, for an SFF Hamiltonian that is LTK-decomposed, given a fixed $\tau > 0$, an $m \in \mathbb{N}$ can be chosen sufficiently large such that $\delta\tau = \tau/m$ is sufficiently small. The inner loop is essentially a multi-dimensional integration over the points $\{q_n : n \in [(i-1)K, (i+1)K]\} \in (\mathcal{C}/A_*)^{2K+1}$ weighted by the Wiener measure $\prod_{n=(i-1)K}^{(i+1)K-1} \langle q_{n+1}|e^{-\delta\tau H_{(n+1)\|K}}|q_n\rangle$, while subject to the constraint that $\langle \mathcal{P}q_{n+1}|e^{-\delta\tau H_{(n+1)\|K}}|\mathcal{P}q_n\rangle$ does not change sign or vanish, $\forall n \in [(i-1)K, (i+1)K-1]$. The Wiener measure is substantially a product between a Gaussian measure representing Brownian motions of free particles and a multiplicative factor valued within the interval $[e^{-2\delta\tau K V_0}, e^{2\delta\tau K V_0}]$, the latter being due to the potential energy terms in the FFIs that are bounded within $[-V_0, V_0]$, $V_0 > 0$. A small $\delta\tau$ dictates that the coordinates $\{q_n : n \in [(i-1)K, (i+1)K]\}$ can not be far separated in the $\mathcal{C}/A_*$ orbifold topology lest the Wiener measure be exponentially small, and each nodal surface can be well approximated locally as a hyperplane bisecting an Euclidean configuration space, for any configuration point q_n, $n \in [(i-1)K, (i+1)K]$ that ever gets close to such a nodal surface. Therefore, the multi-dimensional integration performed by the inner loop is mostly like an MCMC sampling from and integrating a logconcave distribution over a convex polyhedron defined by the hyperplanes locally approximating the nodal surfaces. The latter is proved to mix rapidly [24] with a polynomial-sized Cheeger constant or conductance $CheegConst$ [25–27], so is the former rapidly-mixing with a Cheeger constant no smaller than $e^{-4\delta\tau K V_0} \times CheegConst$.

For each step of the outer loop walking a coordinate $q_{iK} \in \mathcal{C}_{iK}/A_*$, $i \in [0, m]$ to a new position $r_{iK} \in \mathcal{C}_{iK}/A_*$, with all of the other coordinates $\{q_{jK} : j \in [0, m],\, j \neq i\}$ being fixed, the Metropolis-Hastings algorithm or Gibbs sampling accepts or rejects the $q_{iK} \to r_{iK}$ move with a probability that depends on a ratio between two conditional probabilities $\Pr(r_{iK} | \, q^-_{(i+1)K}, q^+_{(i-1)K}) \,/\, \Pr(q_{iK} | \, q^-_{(i+1)K}, q^+_{(i-1)K})$, subject to a constraint that both q_{iK} and r_{iK} can be reached by restricted Feynman paths from both $q^+_{(i-1)K}$ and $q^-_{(i+1)K}$. This is essentially a random walk over a nodal cell of $\Pr(q_{iK} | \, q^-_{(i+1)K}, q^+_{(i-1)K}) \propto \langle \mathcal{P}q^-_{(i+1)K}|e^{-\delta\tau H}|(q_{iK}\rangle \, \langle (q_{iK}|e^{-\delta\tau H}|\mathcal{P}q^+_{(i-1)K}\rangle$ as a function of $q_{iK} \in \mathcal{C}_{iK}/A_*$. The outer loop overall is to drive the distribution of coordinates from an initial $\phi(\{q_{iK}\}_{i\in[0,m]}) \in L^1((\mathcal{C}/A_*)^{m+1})$ to a stationary distribution $\phi_0(\{q_{iK}\}_{i\in[0,m]})$ at equilibrium. To see how fast the process converges, expand the multi-variable function $\phi(\cdot)$ in terms of products among the eigenfunctions $\{\psi_n \stackrel{\text{def}}{=} \psi_n(H)\}_{n\geq 0}$ listed in the order of increasing energies, such that

$$\phi(\{q_{iK} : i \in [0, m]\}) \;=\; \sum\nolimits_{n_0 n_1 \cdots n_m} c_{n_0 n_1 \cdots n_m} \, \psi_{n_0}(q_0)\psi_{n_1}(q_K) \cdots \psi_{n_m}(q_{mK}) \,. \tag{10}$$

Assume that the ground state $\psi_0(H)$ is non-degenerate. Then it is obvious that the equilibrium distribution is precisely $\phi_0(\{q_{iK}\}) = \psi_0(q_0)\psi_0(q_K)\cdots\psi_0(q_{mK})$. Any monomial $\psi_{n_0}(q_0)\cdots\psi_{n_i}(q_{iK})\cdots\psi_{n_m}(q_{mK})$ in equation (10) that has an excited state ψ_{n_i}, $n_i \neq 0$, $i \in [0, m]$ as a factor will have its coefficient $c_{n_0 n_1 \cdots n_m}$ strictly reduced by a factor $e^{-\alpha(i)\delta\tau[\lambda_{n_i}(H) - \lambda_0(H)]} < 1$ after each step of the outer loop walking the coordinate q_{iK}, with $\alpha(0) = \alpha(m) = 1$ and $\alpha(i) = 2$ for all $i \in [1, m-1]$. Therefore, the mixing time [28] of the outer loop is upper-bounded by $O(m/\Delta\lambda)$, with $\Delta\lambda \stackrel{\text{def}}{=} \lambda_1(H) - \lambda_0(H)$ being the spectral gap of H.

Theorem 1. *Let $H = \sum_{k=1}^K H_k$ be an SFF Hamiltonian that is LTK-decomposed, whose ground state is non-degenerate and separated from all excited states by an $\Omega(1/\text{poly}(\text{size}(H)))$ energy gap. Then the Gibbs kernel $\langle \mathcal{P}r|e^{-\tau H}|\mathcal{P}q\rangle$, $(r, q) \in \mathcal{C}^2$ is BPP simulatable for all $\tau \in [0, \infty)$, namely, there is a Monte Carlo algorithm that runs for a time no longer than $\text{poly}(\text{size}(H), \epsilon^{-1})$ to generate a random sample of $(r, q) \in \mathcal{C}^2$, whose probability distribution is no more than ϵ away from $\langle \mathcal{P}r|e^{-\tau H}|\mathcal{P}q\rangle$ in the total variance distance [28], for all $(r, q) \in \mathcal{C}^2$, for any given $\epsilon > 0$.*

Proof. By the exchange symmetry, it is sufficient to simulate the Gibbs kernel $\langle r|e^{-\tau H}|\mathcal{P}q\rangle$ for $q \in \mathcal{C}$ and for $r \in \mathcal{N}(q; \tau H)$, with $\mathcal{N}(q; \tau H)$ denoting the nodal cell of $\langle \cdot|e^{-\tau H}|\mathcal{P}q\rangle$ with respect to and containing a start

point $q \in \mathcal{C}$. Due to the polynomial energy gap, it is WLOG to assume that τ is $O(\text{poly}(\text{size}(H)))$ bounded, because $e^{-\tau[H-\lambda_0(H)]}$ becomes essentially a projection to the ground state when τ is sufficiently large. Employ an MCMC procedure as specified in the above exemplary embodiment, with an m chosen sufficiently large but still $O(\text{poly}(\text{size}(H)))$ bounded, so that $\delta\tau = \tau/m$ is sufficiently small and the inner loop converges well within $O(\text{poly}(\text{size}(H)))$ iterations. Again due to the polynomial energy gap and the uniqueness of $\psi_0(H)$, the outer loop needs to iterate only $\text{poly}(\text{size}(H), \epsilon^{-1})$ times to produce a random sample $(r, q) \in \mathcal{C}^2$ that is distributed ϵ-close to $\langle r|e^{-\tau H}|\mathcal{P}q\rangle$. The overall runtime is clearly $O(\text{poly}(\text{size}(H), \epsilon^{-1}))$. □

Running such an MCMC procedure for a polynomial number of times generates a polynomial number of random samples of $(r, q) \in \mathcal{C}^2$ according to the Gibbs kernel $\langle r|e^{-\tau H}|\mathcal{P}q\rangle$, $q \in \mathcal{C}$, $r \in \mathcal{N}(q; \tau H)$. In particular, by enforcing a periodic boundary condition $r = q_N = q_0 = q$ and running the MCMC for a polynomial number of times, enough samples can be generated to estimate the partition function $Z \stackrel{\text{def}}{=} \int \langle q|e^{-\tau H}|\mathcal{P}q\rangle\, dq$ to within a polynomial accuracy. In general, for any observable Q whose matrix elements $\langle q|Q|r\rangle$, $(q, r) \in \mathcal{C}$ can be efficiently computed, a Feynman slab implementing $\langle q|Q|r\rangle$ can be added to extend a Feynman stack that computes $\langle r|e^{-\tau H}|\mathcal{P}q\rangle$, $(q, r) \in \mathcal{C}$, then the extended Feynman stack can be MCMC simulated, again with the periodic boundary condition enforced, to estimate the expectation value $Z^{-1}\iint \langle q|Q|r\rangle\, \langle r|e^{-\tau H}|\mathcal{P}q\rangle\, dqdr$ to within a polynomial accuracy at the cost of a polynomial runtime. For many applications, there is a contextual prescription to choose a guaranteed warm start $q \in \mathcal{C}$. Alternatively, almost all configuration points are a warm start so long as the Hamiltonian H is well-behaved analytically, *e.g.*, when $H = -\Delta + V$ is of the Schödinger type with a bounded potential V.

For an SFF Hamiltonian $H = \sum_{k=1}^K H_k$ that is GSP-decomposed, it is convenient to adopt the perspective and method of reptation QMC [8, 29–31], where a sequence of Gibbs operators $\{\mathsf{G}_k\}_{k\in[1,K]}$ is applied to a known initial quantum state $|\Phi\rangle$ in turn and repeated for $m \in \mathbb{N}$, $m = O(\text{poly}(\text{size}(H)))$ times, with $\mathsf{G}_k \stackrel{\text{def}}{=} e^{-\delta\tau[H_k-\lambda_0(H_k)]}$, $\forall k \in [1, K]$, $\delta\tau$ being no longer small but sufficiently large such that G_k is essentially the same as $\Pi_k = \lim_{\tau\to\infty} e^{-\tau[H_k-\lambda_0(H_k)]}$ up to an error that is exponentially small, $\forall k \in [1, K]$, and m being sufficiently large such that the projected state $|\Psi\rangle \stackrel{\text{def}}{=} \big(\prod_{k=1}^K \mathsf{G}_k\big)^m|\Phi\rangle$ is essentially the same as $\psi_0(H)$ up to an error this is $O(1/\text{poly}(m))$. For any measurement operator Q of interest, the expectation value $\langle\Psi|Q|\Psi\rangle = \langle\Phi|\big(\prod_{k=1}^K \mathsf{G}_{K-k+1}\big)^m Q\,\big(\prod_{k=1}^K \mathsf{G}_k\big)^m|\Phi\rangle$ can be estimated by RPI with a Feynman stack consisting of $2mK$ Feynman slabs, each of which corresponds to a Gibbs operator G_k, $k \in [1, K]$ and is path rectified in accordance with the nodal structure of the Gibbs kernel $\langle\cdot|\mathsf{G}_k|\cdot\rangle$, which is efficiently computable and readily available in relation to the associated FFI H_k, $\forall k \in [1, K]$. Either Q is coordinate-diagonal, so that $\langle\Psi|Q|\Psi\rangle$ can be computed straightforwardly from a polynomial number of Feynman path samples, or else Q involves a small number of fermion species, and the total Hamiltonian is modified into $H + \eta\, Q$, $\eta \in \mathbb{R}$, which is still SFF, so that an RPI-based reptation QMC is performed for the Hamiltonian $H + \eta\, Q$, from which $\langle\Psi|Q|\Psi\rangle$ is derived by invoking the Feynman-Hellman theorem [29, 31]. In order to ensure a warm start, it is helpful to employ a sequence of SFF Hamiltonians $\mathsf{H}(t) = \sum_{k=1}^K \mathsf{H}_k(t)$, $t \in [0, 1]$, which evolves adiabatically from an easily solvable $\mathsf{H}(0)$ having $|\Phi\rangle$ as its unique ground state to $\mathsf{H}(1) = H$, the target Hamiltonian, such that the Feynman stack associated with the nested sequence of FFIs $\{\{\mathsf{H}_k(t/m)\}_{k\in[1,K]}\}_{t\in[1,m]}$ projects $|\Phi\rangle$ at the start into $|\Psi\rangle = \psi_0(\mathsf{H}(1))$ in the middle [8].

The above method of reptation QMC uses path integral to compute an inner product $\langle\Psi|Q|\Psi\rangle$ for the wavefunction $|\Psi\rangle = \prod_{n=1}^{mK} \mathbf{G}_n|\Phi\rangle$, with $\mathbf{G}_n \stackrel{\text{def}}{=} \mathsf{G}_{n\|K}$, $\forall n \in [1, mK]$. Alternatively, a time-inhomogeneous MCMC can be constructed to compute or sample from the outer (dyadic) product $|\Psi\rangle\langle\Psi|$, that is a density matrix or operator, also called a *Gibbs wavefunction of the second order*. Such time-inhomogeneous MCMC repeats an iterative loop comprising $mK+1$ steps, wherein the zeroth step picks a random sample $|r_0\rangle\langle q_0|$ from a positive nodal cell of $|\Phi\rangle\langle\Phi|$ according to the density function $\Phi(r_0)\Phi(q_0)$, and stores a triple (r_0, q_0, p_0) with $p_0 \stackrel{\text{def}}{=} \Phi(r_0)\Phi(q_0)$ as the initial value of a state variable for the time-inhomogeneous Markov chain; Next, for each $n \in [1, mK]$, the n-th step fixes (r_{n-1}, q_{n-1}) and samples a random dyadic $|r_n\rangle\langle q_n|$ from a positive nodal cell of $\mathbf{G}_n|r_{n-1}\rangle\langle q_{n-1}|\mathbf{G}_n^+$ according to the density function $\langle r_n|\mathbf{G}_n|r_{n-1}\rangle\langle q_{n-1}|\mathbf{G}_n^+|q_n\rangle$, then updates the value of the state variable from $(r_{n-1}, q_{n-1}, p_{n-1})$ to (r_n, q_n, p_n), with $p_n \stackrel{\text{def}}{=} \langle r_n|\mathbf{G}_n|r_{n-1}\rangle\langle q_{n-1}|\mathbf{G}_n^+|q_n\rangle$; In each said n-th step, $n \in [1, mK]$, the density function is efficiently computable and easily path rectified since each $\mathbf{G}_n$, $n \in [1, mK]$ is associated with an FFI; Finally, the mK-th step produces a value (r_{mK}, q_{mK}, p_{mK}) of the state variable, which represents a random sample $|r_{mK}\rangle\langle q_{mK}|$ from $|\Psi\rangle\langle\Psi|$ with a probability weight p_{mK}. Repeating said iterative loop for a polynomial number of times generates an ensemble of samples to

represent $|\Psi\rangle\langle\Psi|$, from which a physical quantity of interest can be derived.

Not only SFF Hamiltonians can be simulated efficiently, but also they are universal for many-body physics and quantum computing. The following will show that any BQP algorithm given as an ordered sequence of *controlled R-gates* [8–10] $\{U_t \stackrel{\text{def}}{=} I \otimes Z_t^+ + R_t \otimes Z_t^-\}_{t\,\in\,[1,T]}$, $T \in \mathbb{N}$ on a quantum computer of $n \in \mathbb{N}$ rebits can be mapped to an LTK- or GSP-decomposed SFF Hamiltonian, where $R_t \stackrel{\text{def}}{=} X \sin\theta(t) + Z\cos\theta(t)$, $\theta(t) \in [-\pi, \pi)$ is a self-inverse gate applied to a rebit indexed by an $i(t) \in [1, n]$, and $Z_t^{\pm}$ are $Z^{\pm} \stackrel{\text{def}}{=} (I \pm Z)/2$ operators applied to a control rebit indexed by a $j(t) \in [1, n]$, $\forall t \in [1, T]$, $X \stackrel{\text{def}}{=} \sigma_x$ and $Z \stackrel{\text{def}}{=} \sigma_z$ are the familiar Pauli matrices acting on a single rebit as the simplest quantum system $(\mathcal{C}_0, \mathcal{H}_0, \mathcal{B}_0)$, with $\mathcal{C}_0 \stackrel{\text{def}}{=} \{0, 1\}$, $\mathcal{H}_0 \stackrel{\text{def}}{=} \{\alpha|0\rangle + \beta|1\rangle : \alpha, \beta \in \mathbb{R}\}$, $\mathcal{B}_0$ being the Banach algebra of 2×2 real matrices. Such a BQP algorithm, or its associated quantum circuit, is said to have a computational size $T + n$.

Definition 3. *A homophysics $\mathfrak{M} : (\mathcal{C}, \mathcal{H}, \mathcal{B}) \mapsto (\mathcal{C}', \mathcal{H}', \mathcal{B}')$ between two quantum systems with Hamiltonians $H \in \mathcal{B}$ and $H' \in \mathcal{B}'$ is an injective mapping that sends any subset $\mathcal{D} \subseteq \mathcal{C}$ to a unique $\mathcal{D}' \stackrel{\text{def}}{=} \mathfrak{M}(\mathcal{D}) \subseteq \mathcal{C}'$, maps any $\psi \in \mathcal{H}$ to a unique $\psi' \stackrel{\text{def}}{=} \mathfrak{M}(\psi) \in \mathcal{H}'$, and sends any $Q \in \mathcal{B}$ to a unique $Q' \stackrel{\text{def}}{=} \mathfrak{M}(Q) \in \mathcal{B}'$, such that $\mathcal{C} \supseteq \mathcal{D} \mapsto \mathfrak{M}(\mathcal{D}) \subseteq \mathcal{C}'$ embeds the Boolean algebra of subsets [32] of $\mathcal{C}$ into the Boolean algebra of subsets of $\mathcal{C}'$; 2) $\mathcal{H} \ni \psi \mapsto \mathfrak{M}(\psi) \in \mathcal{H}'$ embeds the Hilbert space $\mathcal{H}$ into $\mathcal{H}'$; 3) $\mathcal{B} \ni Q \mapsto \mathfrak{M}(Q) \in \mathcal{B}'$ embeds the Banach algebra $\mathcal{B}$ into $\mathcal{B}'$; 4) there exists a constant $c > 0$, $c + c^{-1} = O(\text{poly}(\text{size}(H)))$, with which $\langle\mathfrak{M}(\psi)|\mathfrak{M}(Q)|\mathfrak{M}(\phi)\rangle = c\langle\psi|Q|\phi\rangle$ holds $\forall\psi, \phi \in \mathcal{H}$, $\forall Q \in \mathcal{B}$; 5) $\text{size}(H) = O(\text{poly}(\text{size}(H')))$ and $\text{size}(H') = O(\text{poly}(\text{size}(H)))$. A homophysics $\mathfrak{M}$ is called an isophysics when the mapping $\mathfrak{M}$ is also surjective.*

Firstly, it is useful to construct a bi-fermion system $(\mathcal{C}_1, \mathcal{H}_1, \mathcal{B}_1)$ consisting of two non-interacting identical fermions moving on a circle $\mathbb{T} \stackrel{\text{def}}{=} \mathbb{R}/2\mathbb{Z}$ [8], governed by a single-particle Hamiltonian $-(1/2)\partial^2/\partial x^2 + V(x)$, $x \in \mathbb{T}$, with an external potential $V(x) = V_0\,[d(x, 0) > 1 - a_0]_{\text{Iver}} - V_0\,[d(x, 0) < a_0]_{\text{Iver}}$, $x \in [-1, 1) \pmod 2 \simeq \mathbb{T}$, $a_0 = \gamma_0^{-1}$, $V_0 = \gamma_0^2$, $\gamma_0 \gg 1$ being a large constant, where $d(x, y)$ denotes the geodesic distance between $x \in \mathbb{T}$ and $y \in \mathbb{T}$ along the circle, $[\cdot]_{\text{Iver}}$ is an Iverson bracket [33] which returns a number valued to 1 or 0 depending on if the Boolean expression inside the bracket is true or false. When γ_0 is sufficiently large, the potential well and barrier become essentially Dirac deltas, $V(x) \simeq \gamma_0\delta(x + 1) - \gamma_0\delta(x)$, $x \in [-1, 1) \pmod 2$, such that a bi-fermion under a nominal Hamiltonian $\mathsf{H}_{\text{BF}} = (\gamma_0^2 - \pi^2)/2 + \sum_{i\,=\,1}^{2}[-(1/2)\partial^2/\partial x_i^2 + V(x_i)]$, $(x_1, x_2) \in \mathbb{T}^2$ behaves like a rebit with two low-energy states

$$\psi_+(x_1, x_2) \;=\; (1 - \pi_{12}) \sin\pi[d(x_1, 0) - a_0]\, e^{-\gamma_0 d(x_2, 0)},\ (x_1, x_2) \in [-1, 1)^2, \tag{11}$$

$$\psi_-(x_1, x_2) \;=\; (1 - \pi_{12}) \sin\pi x_1\, e^{-\gamma_0 d(x_2, 0)},\ (x_1, x_2) \in [-1, 1)^2, \tag{12}$$

that are degenerate at $E_0 = 0$, where π_{12} is the fermion exchange operator swapping the particle labels 1 and 2. Choose $\alpha_0 = 2\gamma_0^{-1}\log\gamma_0$, then for all x such that $d(x, 0) > \alpha_0$, the amplitude of the single-particle bound state $|e^{-\gamma_0 d(x,0)}| < \gamma_0^{-2}$, which is rather small. Construct potential functions

$$\mathsf{X}(x_1, x_2) \;=\; \gamma_0\,(1 + \pi_{12})\,[\,d(x_1, 0) > 1 - a_0 \,\wedge\, d(x_2, 0) < \alpha_0\,]_{\text{Iver}} - (\pi^2/4\gamma_0^2)\,, \tag{13}$$

$$\mathsf{Z}^+(x_1, x_2) \;=\; (1 + \pi_{12})\,[\,d(x_1, +1/2) < 1/2 \,\wedge\, d(x_1, 0) > \alpha_0 \,\wedge\, d(x_2, 0) < \alpha_0\,]_{\text{Iver}}\,, \tag{14}$$

$$\mathsf{Z}^-(x_1, x_2) \;=\; (1 + \pi_{12})\,[\,d(x_1, -1/2) < 1/2 \,\wedge\, d(x_1, 0) > \alpha_0 \,\wedge\, d(x_2, 0) < \alpha_0\,]_{\text{Iver}}\,, \tag{15}$$

$\forall(x_1, x_2) \in [-1, 1)^2$. It is clear that a bi-fermion implements a rebit via a homophysics $\mathfrak{M}_1 : (\mathcal{C}_0, \mathcal{H}_0, \mathcal{B}_0) \mapsto (\mathcal{C}_1, \mathcal{H}_1, \mathcal{B}_1)$ such that, with $|\pm\rangle \stackrel{\text{def}}{=} (|0\rangle \pm |1\rangle)/\sqrt{2}$,

$$\mathfrak{M}_1\,(|\pm\rangle \in \mathcal{H}_0) \;=\; \psi_\pm(x_1, x_2) \in \mathcal{H}_1\,, \tag{16}$$

$$\mathfrak{M}_1\,(X \in \mathcal{B}_0) \;=\; (2\gamma_0^2/\pi^2)\,[\mathsf{H}_{\text{BF}} + \mathsf{X}(x_1, x_2)] \in \mathcal{B}_1\,, \tag{17}$$

$$\mathfrak{M}_1\,(Z^\pm \in \mathcal{B}_0) \;=\; \gamma_0\mathsf{H}_{\text{BF}} + \mathsf{Z}^\pm(x_1, x_2) \in \mathcal{B}_1\,. \tag{18}$$

Via linear combinations, the operators $\mathfrak{M}_1(X)$, $\mathfrak{M}_1(Z^+)$, $\mathfrak{M}_1(Z^-)$ generate all partial Hamiltonians that are of interest for quantum computing on a single bi-fermion, because $\text{span}\{X, Z^+, Z^-\}$ contains all Hermitian elements in $\mathcal{B}_0$. It is noted in passing that, although it is preferred for the single-particle potential $V(x)$, $x \in \mathbb{T}$ to have a narrow and deep potential well around $x = 0$, approximating a fairly strong Dirac delta

to localize one of the two fermions in a small neighborhood of $x = 0$, there is no practical necessity other than convenience of mathematical analysis, to require a steep potential barrier around $x = \pm 1$. Rather, it is perfectly fine to place a relatively wide and low potential barrier, as long as its width and height are chosen properly to be commensurate with the Delta-like potential well around $x = 0$, such that the nominal bi-fermion Hamiltonian $H_{\rm BF}$ defines a degenerate two-state Hilbert space implementing a rebit.

Next, it is also straightforward to construct a homophysics $\mathfrak{M}_2 : (\mathcal{C}_0^2, \mathcal{H}_0^2, \mathcal{B}_0^2) \mapsto (\mathcal{C}_1^2, \mathcal{H}_1^2, \mathcal{B}_1^2)$, with $\mathcal{C}_i^2 \stackrel{\rm def}{=} \mathcal{C}_i \times \mathcal{C}_i$, $\mathcal{H}_i^2 \stackrel{\rm def}{=} \mathcal{H}_i \otimes \mathcal{H}_i$, $\mathcal{B}_i^2 \stackrel{\rm def}{=} \mathcal{B}_i \otimes \mathcal{B}_i$, $\forall i \in \{0, 1\}$, so to implement a pair of interacting rebits using two bi-fermions conditioned and interacting through the following partial Hamiltonians,

$$\mathfrak{M}_2 \left(X_1 \otimes Z_2^{\pm} \right) \;=\; (2\gamma_0^2/\pi^2) \left[\, \mathsf{H}_{\rm BF,1} + \mathsf{H}_{\rm BF,2} + \mathsf{X}(x_{11}, x_{12}) \, \mathsf{Z}^{\pm}(x_{21}, x_{22}) \, \right], \tag{19}$$

$$\mathfrak{M}_2 \left(Z_1^{\pm} \otimes Z_2^{\pm} \right) \;=\; \gamma_0 \mathsf{H}_{\rm BF,1} + \gamma_0 \mathsf{H}_{\rm BF,2} + \mathsf{Z}^{\pm}(x_{11}, x_{12}) \, \mathsf{Z}^{\pm}(x_{21}, x_{22}) \, , \tag{20}$$

where $\forall i \in \{1, 2\}$, X_i, $Z_i^{\pm}$, $Z_i = Z_i^+ - Z_i^-$ are the X- and Z-gates on the i-th rebit, $\mathsf{H}_{{\rm BF},i}$ is the nominal Hamiltonian of the i-th bi-fermion, $(x_{i1}, x_{i2}) \in \mathbb{T}^2$ is the two-fermion configuration of the i-th bi-fermion. $X_1 \otimes Z_2^{\pm}$ and $Z_1 \otimes Z_2^{\pm}$ are called *single-rebit-controlled gates*, whose linear combinations include all single-rebit-controlled R gates, which are already universal for ground state quantum computing (GSQC) in the sense that, using the so-called perturbative gadgets, up to an error tolerance $\epsilon > 0$, the low-energy physics of any system of $n \in \mathbb{N}$ rebits under a computationally k-local Hamiltonian, $k \in \mathbb{N}$ being a fixed number, can be homophysically mapped to the low-energy physics of another system of $\text{poly}(n, \epsilon^{-1})$ rebits under a Hamiltonian that involves only one-body and two-body interactions, especially the controlled R-gates, whose operator norms are upper-bounded by $\text{poly}(\epsilon^{-1})$ [10, 34–36]. In particular, the "XX from XZ gadget" of Biamonte and Love [10] can be employed to effect homophysically an $X \otimes X$ interaction between a first and a second rebits through $X \otimes Z$ interactions with a zeroth rebit,

$$\begin{aligned} & I - X_1 \otimes X_2 \\ \stackrel{\mathfrak{M}}{\Longrightarrow} \; & \gamma_0^2 \, (I - X_0) + (I - X_1 \otimes X_2) \\ \stackrel{\mathfrak{M}}{\Longrightarrow} \; & \gamma_0^2 \, (I - X_0) + \gamma_0 \, Z_0 \otimes (X_1 + X_2) + 2I + O(\gamma_0^{-1}) \, , \end{aligned} \tag{21}$$

where $\stackrel{\mathfrak{M}}{\Longrightarrow}$ reads and stands for "is homophysically mapped to", $\gamma_0 \gg 1$ is a large constant. Then the linear combinations of $X \otimes X$ and $Z \otimes X$ include all two-rebit interactions of the form $R(\theta) \otimes X$, with $R(\theta) \stackrel{\rm def}{=} X \sin\theta + Z \cos\theta$, $\theta \in [-\pi, \pi)$. Alternatively, there is a special class of few-rebit interactions called *multi-rebit-controlled gates* of the form $R_i(\theta) \otimes \prod_{j \in J} Z_j^{\pm}$, with $\theta \in [-\pi, \pi)$, i indexing a rebit being operated upon, J being a set indexing a fixed number of control rebits. Such a multi-rebit-controlled R-gate does not require a decomposition into two-rebit couplings, but can be implemented through a linear combination of the following homophysics,

$$\mathfrak{M} \left(X_i \otimes \textstyle\prod_{j \in J} Z_j^{\pm} \right) \;=\; (2\gamma_0^2/\pi^2) \left[\, \mathsf{H}_{{\rm BF},i} + \sum_{j \in J} \mathsf{H}_{{\rm BF},j} + \mathsf{X}(x_{i1}, x_{i2}) \prod_{j \in J} \mathsf{Z}^{\pm}(x_{j1}, x_{j2}) \, \right], \tag{22}$$

$$\mathfrak{M} \left(Z_i^{\pm} \otimes \textstyle\prod_{j \in J} Z_j^{\pm} \right) \;=\; \gamma_0 \mathsf{H}_{{\rm BF},i} + \gamma_0 \sum_{j \in J} \mathsf{H}_{{\rm BF},j} + \mathsf{Z}^{\pm}(x_{i1}, x_{i2}) \prod_{j \in J} \mathsf{Z}^{\pm}(x_{j1}, x_{j2}) \, . \tag{23}$$

At any rate, it has been established that any computationally k-local Hamiltonian H involving $n \in \mathbb{N}$ rebits, with $k \in \mathbb{N}$ being a fixed number and n a variable, can be homophysically implemented as an SFF Hamiltonian $\mathfrak{M}(H)$ involving no more than $\text{poly}(n, \epsilon^{-1})$ bi-fermions, such that the low-energy physics of H and $\mathfrak{M}(H)$ are homophysical up to a variable error tolerance $\epsilon > 0$, where each FFI in $\mathfrak{M}(H)$ moves no more than $k' \in \mathbb{N}$ bi-fermions, with k' being another fixed number, and has an operator norm that is upper-bounded by $\text{poly}(\epsilon^{-1})$, while all bi-fermions are mutually distinguishable entities.

Given a universal BQP algorithm $\{U_t \stackrel{\rm def}{=} I \otimes Z_t^+ + R_t \otimes Z_t^-\}_{t \in [1,T]}$, $T \in \mathbb{N}$, with each controlled R-gate U_t operating on an $i(t)$-th, $i(t) \in [1, n]$ and a $j(t)$-th, $j(t) \in [1, n]$ rebits in an n-rebit *logic register* represented by $(\mathcal{C}_L \stackrel{\rm def}{=} \{0, 1\}^n, \mathcal{H}_L, \mathcal{B}_L)$ as a quantum subsystem, each R_t being self-inverse, $\forall t \in [1, T]$, where the successive applications of the controlled-R gates are meant to generate a series of quantum states $|\phi_t\rangle_L \stackrel{\rm def}{=} U_t |\phi_{t-1}\rangle_L$, $t \in [1, T]$, from a given initial state $|\phi_0\rangle_L$ till a computational result $|\phi_T\rangle_L = \big(\prod_{t=1}^{T} U_t \big) |\phi_0\rangle_L$ at the end, the celebrated Feynman-Kitaev construct [3, 8, 11, 12] introduces a *clock register* represented by $(\mathcal{C}_C, \mathcal{H}_C, \mathcal{B}_C)$ as a

quantum subsystem to support *clock states* $\{|t\rangle_C\}_{t\in[0,T]} \subseteq \mathcal{H}_C$, so that the clock and logic registers constitute a GSQC system represented by $(\mathcal{C}_C \times \mathcal{C}_L, \mathcal{H}_C \otimes \mathcal{H}_L, \mathcal{B}_C \otimes \mathcal{B}_L)$, on which the product states $\{|t\rangle_C|\phi_t\rangle_L\}_{t\in[0,T]} \subseteq \mathcal{H}_C \otimes \mathcal{H}_L$ map and encode the entire computational history of the BQP algorithm. Then Feynman's clocked Hamiltonians $H_{\text{Feyn},\,t} \stackrel{\text{def}}{=} |t\rangle_C\langle(t-1)|_C \otimes U_t + |(t-1)\rangle_C\langle t|_C \otimes U_t$, $t \in [1,T]$ ensure that the associated quantum gates U_t, $t \in [1,T]$ are applied to the logic register in the correct order when the clock register undergoes transitions between what he called the *program counter sites* (namely, the clock states) $|t\rangle_C$, $t \in [1,T]$ [3]. Finally, Kitaev's GSQC Hamiltonian (also called the *Feynman-Kitaev Hamiltonian*) $H_{\text{FK}} \stackrel{\text{def}}{=} H_{\text{clock}} + H_{\text{init}} + H_{\text{prop}}$ enforces computational constraints via energy penalties, with H_{clock} restricting the clock register to the manifold of $\text{span}(\{|t\rangle_C : t \in [0,T]\})$, H_{init} setting the initial state, while H_{prop} performing the quantum computation as Feynman suggested, such that the ground state $\psi_0(H_{\text{FK}}) = (T+1)^{-1/2}\sum_{t=0}^{T}|t\rangle_C|\phi_t\rangle_L$ is unique and polynomially gapped [11, 12].

There are several choices of encoding a clock register for the clock states $\{|t\rangle_C\}_{t\in[0,T]}$ [37, 38]. Take Kitaev's *domain wall clock* for example, which has a clock register consisting of $T+2$ rebits indexed by integers within $[0, T+1]$, and uses $|t\rangle_C \stackrel{\text{def}}{=} |1\rangle_C^{\otimes(t+1)}|0\rangle_C^{\otimes(T-t+1)}$, $t \in [0,T]$, such that [8, 11, 12]

$$H_{\text{FK}} \stackrel{\text{def}}{=} H_{\text{clock}} + H_{\text{init}} + \sum_{t=1}^{T} H_{\text{prop},\,t}\,, \tag{24}$$

$$H_{\text{clock}} \stackrel{\text{def}}{=} Z^{+}_{C,\,0} + Z^{-}_{C,\,T+1} + \sum_{t=1}^{T} Z^{+}_{C,\,t-1} \otimes Z^{-}_{C,\,t}\,, \tag{25}$$

$$H_{\text{init}} \stackrel{\text{def}}{=} Z^{+}_{C,\,1} \otimes (I - |\phi_0\rangle_L\langle\phi_0|_L)\,, \tag{26}$$

$$H_{\text{prop},\,t} \stackrel{\text{def}}{=} Z^{-}_{C,\,t-1} \otimes Z^{+}_{C,\,t+1} \otimes (I - X_{C,\,t} \otimes U_t)\,,\ \forall t \in [1,T]\,, \tag{27}$$

where $Q^{\delta}_{C,\,t}$ means to apply a single-rebit operator Q^{δ} to the t-th rebit of the clock register, $\forall Q \in \{X, Z\}$, $\forall \delta \in \{+, -, \text{void}\}$, $\forall t \in [0, T+1]$. The partial Hamiltonians $\{H_{\text{prop},\,t}\}_{t\in[1,T]}$ are called the *Feynman-Kitaev propagators*. It is clear that $\text{size}(H_{\text{FK}}) = O(T+n)$. It is WLOG to assume that the initial state $|\phi_0\rangle_L\langle\phi_0|_L$ is $\mathcal{C}_L$-diagonal, because, otherwise, $|\phi_0\rangle_L$ must be preparable from a $\mathcal{C}_L$-coordinate eigenstate by another BQP algorithm. It is straightforward to implement such an H_{FK} into an $\mathfrak{M}(H_{\text{FK}})$ for a system of $2T+n+2$ bi-fermions, where each of the $T+2$ clock rebits and n logic rebits corresponds to one unique bi-fermion, each of the operator monomials in equations (25) and (26) is mapped straightforwardly to an interaction among the corresponding bi-fermions as in equation (23), while the remaining T bi-fermions supply enough auxiliary rebits for perturbative gadgets to implement logic gates of the form $R(\theta) \otimes X$, $\theta \in [-\pi, \pi)$ that may appear in an operator monomial of equation (27).

Theorem 2. *A homophysics $\mathfrak{M}$ exists, which maps the Feynman-Kitaev Hamiltonian H_{FK} as defined in equations (24-27) to an SFF Hamiltonian $\mathfrak{M}(H_{\text{FK}})$ that is both LTK- and GSP-decomposed.*

Proof. An $\mathfrak{M}(H_{\text{FK}})$ as constructed above is obviously SFF, with each FFI corresponding to one of the operator monomials in equations (25-27), each FFI involving no more than 6 bi-fermions and moving even less. Such an SFF Hamiltonian is clearly LTK-decomposed, which also happens to be GSP-decomposed, because H_{FK} is frustrate-free [8, 11, 12, 39, 40], so is $\mathfrak{M}(H_{\text{FK}})$. □

Theorem 3. *BQP ⊆ BPP, therefore BPP = BQP, as BPP ⊆ BQP is well known.*

Proof. By Theorem 2, any BQP algorithm of size $N \in \mathbb{N}$ can be mapped to an SFF Hamiltonian $\mathfrak{M}(H_{\text{FK}})$ with $\text{size}(\mathfrak{M}(H_{\text{FK}})) = O(\text{poly}(N))$, which is both LTK- and GSP-decomposed, as well as polynomially energy gapped. Theorem 1 says that such an $\mathfrak{M}(H_{\text{FK}})$ can be efficiently simulated via Monte Carlo on a classical computer, hence BQP ⊆ BPP. □

In conclusion, it has been proved that BPP and BQP are exactly the same computational complexity class. As a consequence, any quantum system can be efficiently simulated via Monte Carlo on a classical computer, by just constructing a BQP algorithm simulating the quantum system, then mapping the BQP algorithm to an efficient MCMC through a Feynman-Kitaev construct.

Finally, it is useful to note that the analyses, algorithms, and methods presented *supra* can be extended straightforwardly to physical and computational systems over a discrete or continuous-discrete product configuration space [8], only that the nodal restriction or path rectification may need to invoke the so-called *lever rule* [8, 41, 42] using efficiently solved nodal structures of FFIs or their associated Gibbs kernels.

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