Hamiltonian of Mean Force: Exact Influence Functional and Operator Locality Criterion

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Abstract goes here.

INTRODUCTION

In closed quantum statistical mechanics, equilibrium is generated by a Hamiltonian: $\rho \propto e^{-\beta H}$. For an open system with finite coupling, the operationally defined equilibrium state of the subsystem is the reduced state of the global Gibbs ensemble,

$$\bar{\rho}_S(\beta) = \mathrm{Tr}_B\, e^{-\beta H_{\mathrm{tot}}}, \tag{1}$$

$$e^{-\beta H_{\mathrm{MF}}(\beta)} \propto \frac{\mathrm{Tr}_B e^{-\beta H_{\mathrm{tot}}}}{Z_B(\beta)}, \quad Z_B(\beta) = \mathrm{Tr}_B e^{-\beta H_B}. \tag{2}$$

This object is generally not $e^{-\beta H_Q}$ for the bare system Hamiltonian H_Q. The resulting representational question is precise: what operator, if any, plays the role of an equilibrium generator for the subsystem once the coupling is non-negligible? The Hamiltonian of mean force (HMF) answers this by construction and is the standard starting point in strong-coupling thermodynamics and the mean-force Gibbs-state program [1–4].

Why care about a mean-force Hamiltonian at all? First, it provides the exact reduced equilibrium object that underlies strong-coupling thermodynamic identities, including free-energy and work relations that remain valid beyond weak coupling[1, 4, 5]. Second, it furnishes a consistent equilibrium initialization for open-system dynamics when correlations with the bath are unavoidable, a point emphasized in the literature on correlated initial states and reduced dynamics [3, 6]. Related subensemble approaches explicitly treat the subsystem thermodynamics as inherited from a global canonical ensemble, making the effective reduced generator central to the formalism[7]. In short, the HMF is not an optional reinterpretation; it is the exact operator that encodes the reduced equilibrium state whenever system–bath coupling is finite.

Historically, open-system theory prioritized weak-coupling and Markovian regimes, where reduced equilibrium can often be approximated by a Gibbs state of a renormalized H_Q. At finite coupling the reduced state inherits explicit temperature dependence and interaction-induced operator content that is not captured by a simple renormalization. Coupling-dependent thermodynamic response features in quantum Brownian motion and related models highlight this complexity[8, 9]. The strong-coupling literature consequently treats the mean-force Gibbs state as a distinct equilibrium object, with operational ramifications for heat and energy definitions[10, 11].

The HMF literature itself is broad but structured. Canonical definitions and thermodynamic identities are developed in strong-coupling thermodynamics and fluctuation-relation work[1, 2, 4, 5]. A comprehensive review consolidates the "static" mean-force Gibbs perspective with the "dynamical" return-to-equilibrium perspective in open quantum systems [3]. Operational questions such as measurability and thermodynamic consistency at strong coupling have also been pursued[11, 12].

Exact or controlled evaluations exist in special cases. For commuting (QND) interactions, the operator algebra closes trivially and the HMF can be written explicitly[13]. Quadratic/Gaussian models (e.g., damped harmonic oscillators) are solvable because Gaussianity is preserved, leading to closed operator forms[14–16]. Finite-dimensional closures such as spin-boson or single-qubit models provide additional controlled benchmarks[17]. Beyond these cases, the mean-force Gibbs state is often accessed through systematic limits: Cresser and Anders derive weak- and ultrastrong-coupling expressions and show that, in the ultrastrong limit, the mean-force Gibbs state becomes diagonal in the interaction basis rather than the system Hamiltonian basis[18]. Recent work generalizes the HMF framework to finite baths by introducing a pair of quantum Hamiltonians of mean force that incorporate bath feedback[19], and structural studies further analyze the operator content of the HMF in extended settings[20].

Outside solvable models, most approaches are perturbative or numerical. Weak-coupling/high-temperature expansions yield controlled but limited series[18]. Imaginary-time path-integral methods, stochastic representations, and hierarchical-equations techniques can compute $\rho_S(\beta)$ directly but typically do not provide a compact operator form for H_{MF}[21–25]. Stochastic Liouville and partition-free approaches provide complementary numerical access to open-system equilibration without yielding closed-form HMFs [26, 27]. These methods are indispensable for quantitative predictions but leave open the representational question: when does a local or otherwise restricted operator form exist?

The influence-functional formalism is a natural language for this problem. For Gaussian baths with linear coupling it provides an exact route to integrating out bath degrees of freedom[14, 15, 28]. In equilibrium it becomes a Euclidean (imaginary-time) influence functional, usually bilocal in τ, and admits a Hubbard–Stratonovich rewriting as a quenched Gaussian-field average[29–31]. Related path-integral derivations of quantum Langevin dynamics make explicit the noise and dissipation structure inherited from the bath[32, 33]. This formulation also clarifies the terminology: "nonlocal" initially refers to imaginary-time nonlocality of the kernel, whereas the HMF locality question concerns the operator structure on the system Hilbert space.

The existence of $H_{\rm MF}$ is therefore not the issue—it is defined by a logarithm of a traced exponential. The real obstruction is representability: when does $H_{\rm MF}$ admit a closed-form expression within a restricted operator family (few-body, spatially local, or a given algebra)? Much of the literature either (i) solves special models, (ii) expands in controlled limits, or (iii) computes $\rho_S(\beta)$ numerically and analyzes its properties, but a general structural criterion is still lacking [18–20].

This paper provides an exact structural reformulation of the reduced equilibrium operator for Gaussian baths with linear coupling, written both as an imaginary-time influence functional and as a quenched Gaussian-field average. We then organize the operator content by the adjoint-action hierarchy and Magnus/BCH/Lie-factorization language to state an explicit closure criterion: a closed-form local HMF exists only when the operator algebra generated by repeated adjoint action of H_Q on the coupling operators closes inside the target ansatz. The analysis is anchored by minimal solvable examples (commuting coupling, quadratic/Gaussian models, single qubit), and broader implications are deferred.

THEORETICAL DERIVATION

This section derives an exact operator expression for the reduced equilibrium object and provides a systematic criterion for when it admits a local Hamiltonian representation. No weak-coupling or Markovian assumptions are introduced. The only structural assumption is a Gaussian bath with linear coupling, which makes the influence functional bilocal and exact.

Definitions and reduced equilibrium operator

We consider a composite Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ and total Hamiltonian

$$H_{\rm tot} = H_Q + H_B + H_I, \qquad H_I = f \otimes B, \tag{3}$$

where H_Q acts on the system, H_B on the bath, and the interaction is bilinear for clarity. (A sum $\sum_j f_j \otimes B_j$ is treated by the same steps with a matrix-valued kernel.) The unnormalized reduced equilibrium operator is

$$\bar{\rho}_S(\beta) = {\rm Tr}_B\, e^{-\beta H_{\rm tot}}, \tag{4}$$

with normalized state

$$\rho_S = \frac{\bar{\rho}_S}{{\rm Tr}_S \bar{\rho}_S}. \tag{5}$$

The Hamiltonian of mean force (HMF) is defined by

$$e^{-\beta H_{\rm MF}(\beta)} = \frac{{\rm Tr}_B\, e^{-\beta(H_Q+H_B+H_I)}}{Z_B(\beta)}, \qquad Z_B(\beta) = {\rm Tr}_B e^{-\beta H_B}, \tag{6}$$

up to an additive scalar fixed by ${\rm Tr}_S e^{-\beta H_{\rm MF}}$. This operator definition is standard in strong-coupling thermodynamics and is exact[1–4].

Imaginary-time interaction picture and exact Dyson identity

Split $H_{\rm tot} = H_0 + H_I$ with $H_0 = H_Q + H_B$. Define the imaginary-time interaction-picture propagator

$$U(\tau) \equiv e^{\tau H_0} e^{-\tau H_{\rm tot}}, \qquad U(0) = \mathbb{I}. \tag{7}$$

Differentiating and using $H_{\rm tot} = H_0 + H_I$ gives the exact evolution

$$\frac{d}{d\tau} U(\tau) = -\tilde{H}_I(\tau)\, U(\tau), \qquad \tilde{H}_I(\tau) = e^{\tau H_0} H_I e^{-\tau H_0}, \tag{8}$$

whose solution is the ordered exponential

$$U(\beta) = \mathcal{T}_\tau \exp\left(-\int_0^\beta d\tau\, \tilde{H}_I(\tau)\right). \tag{9}$$

Therefore,

$$e^{-\beta H_{\rm tot}} = e^{-\beta H_0}\, \mathcal{T}_\tau \exp\left(-\int_0^\beta d\tau\, \tilde{H}_I(\tau)\right), \tag{10}$$

which is the standard imaginary-time Dyson identity [14, 15, 28]. Since H_0 is a sum of commuting system and bath Hamiltonians, $\tilde{H}_I(\tau) = \tilde{f}(\tau) \otimes \tilde{B}(\tau)$ with

$$\tilde{f}(\tau) = e^{\tau H_Q} f e^{-\tau H_Q}, \qquad \tilde{B}(\tau) = e^{\tau H_B} B e^{-\tau H_B}. \tag{11}$$

Gaussian bath trace and bilocal influence functional

Using $e^{-\beta H_0} = e^{-\beta H_Q} e^{-\beta H_B}$, the bath trace becomes

$$\bar{\rho}_S = e^{-\beta H_Q} \left\langle \mathcal{T}_\tau \exp\left(-\int_0^\beta d\tau\, \tilde{f}(\tau)\tilde{B}(\tau)\right)\right\rangle_B, \tag{12}$$

where $\langle\cdot\rangle_B \equiv \mathrm{Tr}_B(\cdot\,\rho_B)$ and $\rho_B = Z_B^{-1} e^{-\beta H_B}$. A cumulant expansion for the ordered exponential gives

$$\left\langle \mathcal{T}_\tau \exp\left(-\int d\tau\, \tilde{f}(\tau)\tilde{B}(\tau)\right)\right\rangle_B$$
$$= \exp\left(\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int d\tau_1 \cdots d\tau_n\, C_n(\tau_1,\ldots,\tau_n) \prod_{j=1}^{n} \tilde{f}(\tau_j)\right), \tag{13}$$

with cumulants

$$C_n(\tau_1,\ldots,\tau_n) \equiv \langle \mathcal{T}_\tau \tilde{B}(\tau_1)\cdots\tilde{B}(\tau_n)\rangle_c. \tag{14}$$

For a Gaussian bath (e.g., a harmonic bath with linear coupling), all cumulants beyond second order vanish, yielding the exact bilocal influence functional

$$\bar{\rho}_S = e^{-\beta H_Q}\, \mathcal{T}_\tau \exp\Bigg(-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \; \tilde{f}(\tau)\, K(\tau-\tau')\, \tilde{f}(\tau')\Bigg), \tag{15}$$

where the thermal kernel is

$$K(\tau-\tau') \equiv \langle \mathcal{T}_\tau \tilde{B}(\tau)\tilde{B}(\tau')\rangle_B. \tag{16}$$

This form is standard for linear coupling to Gaussian baths and is exact under that assumption[14, 15, 24, 25, 28]. The ordering operator remains because the system operators at different imaginary times need not commute.

Gaussian-field (Hubbard–Stratonovich) reformulation

The bilocal quadratic form in Eq. (15) can be linearized exactly by a Hubbard–Stratonovich transformation. Introducing a real Gaussian field $\xi(\tau)$ with covariance $\langle \xi(\tau)\xi(\tau')\rangle = K(\tau-\tau')$, one obtains

$$\bar{\rho}_S = e^{-\beta H_Q} \left\langle \mathcal{T}_\tau \exp\left(-\int_0^\beta d\tau\, \xi(\tau)\tilde{f}(\tau)\right)\right\rangle_\xi. \tag{17}$$

This "quenched" Gaussian average is an exact operator identity and is widely used in stochastic unravellings and equilibrium reduced-density formulations [21, 22, 27, 29–31]. The associated imaginary-time evolution equation for the ordered exponential is made explicit in Appendix .

Time ordering and interaction-picture dynamics of f

Although f is time independent in the Schrödinger picture, the interaction-picture operator $\tilde{f}(\tau)$ is nontrivial whenever $[H_Q, f] \neq 0$. Differentiating Eq. (11) yields

$$\frac{d}{d\tau}\tilde{f}(\tau) = [H_Q, \tilde{f}(\tau)], \qquad \tilde{f}(0) = f, \tag{18}$$

so the ordered product $\mathcal{T}_\tau \tilde{f}(\tau)\tilde{f}(\tau')$ cannot be reduced to f^2 unless $[H_Q, f] = 0$. Ordered-exponential calculus and the resulting commutator hierarchy are standard; see Refs. [34–36].

Adjoint-action expansion and kernel moments

Define the adjoint action $\mathrm{ad}_{H_Q}(X) = [H_Q, X]$ and its iterates. The interaction-picture operator admits the exact expansion

$$\tilde{f}(\tau) = e^{\tau \mathrm{ad}_{H_Q}}(f) = \sum_{n=0}^{\infty} \frac{\tau^n}{n!}\, \mathrm{ad}_{H_Q}^n(f), \tag{19}$$

which follows from the exponential map for operator adjoint actions [34]. Substituting into the bilocal exponent in Eq. (15) yields the exact algebraic expansion

$$\int_0^\beta d\tau \int_0^\beta d\tau'\, K(\tau-\tau')\, \tilde{f}(\tau)\tilde{f}(\tau') = \sum_{n,m=0}^{\infty} \mu_{nm}\, \mathrm{ad}_{H_Q}^n(f)\, \mathrm{ad}_{H_Q}^m(f), \tag{20}$$

with kernel moments

$$\mu_{nm} \equiv \frac{1}{n!\,m!} \int_0^\beta d\tau \int_0^\beta d\tau'\, \tau^n (\tau')^m K(\tau-\tau'). \tag{21}$$

This separates bath statistics (in μ_{nm}) from the system operator algebra. Symmetry properties of K and relations among μ_{nm} are given in Appendix .

Exact closure criterion and local construction

Define the adjoint-generated subspace

$$\mathcal{A}_f = \mathrm{span}\{\mathrm{ad}_{H_Q}^n(f)\}_{n=0}^{\infty}. \tag{22}$$

The influence functional in Eq. (15) is an ordered exponential built from products of elements of $\mathcal{A}_f$. Consequently, **an exact local Hamiltonian of mean force exists as a finite operator polynomial if and only if the associative algebra generated by $\mathcal{A}_f$ (together with the identity) is finite dimensional and closed under multiplication**. Equivalently, the Lie algebra generated by $\mathcal{A}_f$ is finite dimensional, and the corresponding Magnus/BCH series for the logarithm of the ordered exponential closes within its enveloping algebra[35–38].

When the closure condition holds, one may write

$$\mathcal{T}_\tau \exp\left(-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\, \tilde{f}(\tau)\, K(\tau-\tau')\, \tilde{f}(\tau')\right) = e^{\Omega}, \tag{23}$$

with Ω a finite linear combination of basis elements in the closed algebra (Magnus expansion). Combining $e^{-\beta H_Q}$ with e^{Ω} via the Baker–Campbell–Hausdorff formula yields $\bar{\rho}_S = e^{-\beta H_{\mathrm{MF}}}$ with H_{MF} in the same operator class. When closure fails, the Magnus/BCH series does not truncate and any finite local ansatz for H_{MF} necessarily requires truncation or projection; this is the only point where approximation enters.

METHODS

This section summarizes a concrete procedure for determining whether the HMF can be represented within a local operator class and for constructing it when closure holds.

Step 1: Adjoint chain. Compute the adjoint sequence $\{\mathrm{ad}^n_{H_Q}(f)\}_{n\geq 0}$ until linear dependence is observed. If the span stabilizes after N steps, record a basis $\{O_1, \ldots, O_N\}$ for $\mathcal{A}_f$.

Step 2: Algebraic closure. Check whether the associative products $O_i O_j$ can be expressed within the same finite basis (together with the identity). If so, the generated operator algebra is finite dimensional and closed under multiplication. This is the exact closure criterion of Sec. . Lie-algebraic closure of $\{O_i\}$ implies that the Magnus/BCH series for the ordered exponential closes within the finite enveloping algebra [35–37].

Step 3: Kernel moments. Compute the kernel moments μ_{nm} from Eq. (21) using the bath correlation function $K(\tau - \tau')$. For harmonic baths, K is determined by the spectral density and temperature [15, 24].

Step 4: Construct H_{MF}. With the basis and moments in hand, assemble the bilocal exponent via Eq. (20), write the ordered exponential as $\exp(\Omega)$ using the Magnus expansion, and combine with $e^{-\beta H_Q}$ using BCH. When the algebra closes, H_{MF} is a finite operator polynomial. When it does not, any truncation or projection is the sole source of approximation.

RESULTS: ANALYTIC EXAMPLES

We provide three minimal analytic examples that illustrate the closure criterion and its consequences. These examples are not approximations; they serve only to show when closure is exact.

Commuting coupling

If $[H_Q, f] = 0$, then $\mathrm{ad}^n_{H_Q}(f) = 0$ for all $n \geq 1$, so $\tilde{f}(\tau) = f$ and the time ordering becomes trivial. The bilocal exponent reduces to a scalar multiple of f^2, and the HMF is exactly local. This is the simplest solvable case and is consistent with known exactly solvable strong coupling models[13].

Quadratic/Gaussian system

Consider a harmonic system with $H_Q = p^2/2m + (1/2)m\omega^2 q^2$ and linear coupling $f = q$. The adjoint action closes on the finite set $\{q, p, \mathbb{I}\}$ since $[H_Q, q] \propto p$ and $[H_Q, p] \propto q$. Consequently, the associative algebra generated by $\mathcal{A}_f$ is finite dimensional and the HMF is a quadratic operator. This reproduces the known Gaussian character of the reduced equilibrium state and its mean-force Hamiltonian in damped harmonic models[15, 16].

Single qubit (Pauli algebra)

Let $H_Q = (\omega/2)\sigma_z$ and $f = \sigma_x$. Then $\mathrm{ad}_{H_Q}(f) = \omega i \sigma_y$ and $\mathrm{ad}^2_{H_Q}(f) = -\omega^2 \sigma_x$, so the adjoint chain closes on the Pauli algebra $\{\sigma_x, \sigma_y, \sigma_z, \mathbb{I}\}$. Hence the closure criterion is satisfied and H_{MF} lies in the same finite operator class. This is consistent with standard spin-boson constructions[17].

DISCUSSION

We have derived an exact operator reformulation of the reduced equilibrium object for a Gaussian bath, expressed both as a bilocal imaginary-time influence functional and as a quenched Gaussian-field average. The nonlocal structure in imaginary time is traced entirely to noncommutativity between H_Q and the coupling operator f, which forces the interaction-picture operator $\tilde{f}(\tau)$ to appear in time-ordered products. By expanding $\tilde{f}(\tau)$ in adjoint actions and isolating kernel moments, we obtained a purely algebraic representation that yields an exact closure criterion for locality of H_{MF}.

When the adjoint-generated operator algebra closes, the mean-force Hamiltonian is a finite operator polynomial and can be constructed via Magnus/BCH. When it does not, any local representation necessarily involves truncation or projection; no other approximation is introduced. Broader implications of these results are deferred.

Quenched Density and Imaginary-Time Evolution

This appendix makes explicit the operator identity underlying the quenched imaginary-time formulation used in Sec. . Define a time-ordered exponential with a (generally) τ-dependent operator $H(\tau)$,

$$\begin{aligned} \rho(\tau) &\equiv \mathcal{T}_\tau \exp\left(-\int_0^\tau d\tau'\, H(\tau')\right), \\ \rho(0) &= \mathbb{I}. \end{aligned} \tag{24}$$

Standard differentiation identities for ordered exponentials imply

$$-\partial_\tau \rho(\tau) = H(\tau)\rho(\tau), \tag{25}$$

with the ordering built into $\rho(\tau)$; see, e.g., Refs. [34–36] for operator calculus and time-ordered exponentials.

In the present context one takes

$$H(\tau) = H_Q + \xi(\tau) f, \tag{26}$$

where the Gaussian field satisfies

$$\langle \xi(\tau)\xi(\tau')\rangle = K(\tau - \tau'). \tag{27}$$

The reduced equilibrium operator can be written as

$$\bar{\rho}_S = e^{-\beta H_Q} \langle \rho(\beta)\rangle_\xi\,, \tag{28}$$

which is the compact operator form of the quenched Gaussian representation used in the main text.

To connect Eq. (28) to an imaginary-time path integral, one discretizes $\tau \in [0, \beta]$, applies a Trotter (or Zassenhaus) factorization, and inserts resolutions of identity in the system coordinate basis. This yields the standard Euclidean path-integral expression for the canonical density operator, with the τ-dependent potential induced by the auxiliary field, as in the influence-functional derivation for quadratic baths and their stochastic unravellings [14, 15, 21, 22, 28].

Kernel Symmetry and Moment Relations

The bath kernel appearing in the bilocal influence functional is

$$\begin{aligned} K(\tau - \tau') &= \mathrm{Tr}_B\left[\mathcal{T}_\tau \tilde{B}(\tau)\tilde{B}(\tau')\rho_B\right], \\ \rho_B &= \frac{e^{-\beta H_B}}{Z_B}. \end{aligned} \tag{29}$$

For equilibrium baths, K depends only on the imaginary-time difference and is even under exchange of its arguments, implying

$$K(\tau - \tau') = K(\tau' - \tau), \qquad \mu_{nm} = \mu_{mn}, \tag{30}$$

where μ_{nm} are the kernel moments defined in Eq. (21). In common quadratic-bath models the kernel is explicitly constructed from the bath spectral density and satisfies the Kubo-Martin-Schwinger periodicity in imaginary time, which can be used to re-express moment integrals in equivalent forms; see Refs. [15, 24, 25] for explicit constructions.

The moment expansion used in Sec. requires only these symmetry properties and the existence of the integrals defining μ_{nm}. No further approximation is introduced at this stage.

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