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,

$$\rho_S^{\mathrm{unnorm}}(\beta) = \mathrm{Tr}_B\, e^{-\beta H_{\mathrm{tot}}}, \tag{1}$$

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

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[1–4].

Historically, much of open-system theory emphasized weak-coupling and Markovian regimes, where reduced equilibrium states are well approximated by Gibbs states of renormalized system Hamiltonians. At finite coupling, equilibrium consistency is anchored in the correlated global Gibbs state, and the reduced operator inherits coupling-dependent structure that need not be captured by a simple renormalization. The HMF can become temperature dependent and can encode interaction-induced terms that are absent in H_Q, including effective many-body or nonlocal operator content[2, 4–8]. This is the conceptual tension: the reduced equilibrium state is well defined, but its generator is not generally simple.

The literature on H_{MF} has developed along several lines. Canonical definitions appear in strong-coupling thermodynamics and fluctuation relations, where H_{MF} is tied to partition functions, free energies, and thermodynamic identities[1, 2, 4, 9, 10]. Related work examines measurability and operational meaning in the presence of finite coupling[3, 11, 12]. Exact or controlled computations are available in special models: commuting (QND-type) couplings where the operator algebra closes trivially [13], quadratic/Gaussian systems such as the damped harmonic oscillator where Gaussianity is preserved [14–16], and finite-dimensional closures such as spin-boson or single-qubit settings [17]. Recent work also investigates structural aspects and generalized definitions of H_{MF} beyond these solvable cases[18, 19].

Outside solvable models, most approaches are perturbative or numerical. Weak-coupling and high-temperature expansions yield controlled but limited series[20], while semiclassical limits require additional structure that is model dependent[2]. Operator expansions proliferate under nested commutators, and truncations can be difficult to justify a priori. Numerical approaches based on imaginary-time path integrals and HEOM compute $\rho_S(\beta)$ directly but do not typically yield a compact operator expression for H_{MF}[21–25]. These methods are essential for quantitative results, but they do not resolve the representational question: when is a closed-form local generator available?

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, 26]. In equilibrium this becomes a Euclidean (imaginary-time) influence functional that is bilocal in τ and can be rewritten as a quenched Gaussian-field average via Hubbard–Stratonovich transformations [21, 22, 27–29]. This formulation clarifies an important distinction: "nonlocal" initially means nonlocal in imaginary time through the kernel, whereas the locality question for H_{MF} concerns the operator structure on the system Hilbert space.

The existence of H_{MF} is not the issue—it is defined by a logarithm of a traced exponential. The real obstruction is representability: when does H_{MF} admit a closed-form expression within a restricted operator family (for example, few-body or spatially local Hamiltonians)? Most of the literature either (i) solves special models, (ii) expands perturbatively, or (iii) computes $\rho_S(\beta)$ numerically and studies its properties [18–20]. What is missing is an exact structural reformulation that makes the obstruction explicit and checkable.

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. We impose no weak-coupling or Markovian assumptions. 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

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

where H_Q acts on the system, H_B on the bath, and the interaction is bilinear for clarity. The unnormalized reduced equilibrium operator is

$$\rho_S^{\text{unnorm}}(\beta) = \mathrm{Tr}_B\, e^{-\beta H_{\text{tot}}}, \tag{4}$$

with normalized state

$$\rho_S = \frac{\rho_S^{\text{unnorm}}}{\mathrm{Tr}_S \rho_S^{\text{unnorm}}}. \tag{5}$$

The Hamiltonian of mean force is defined by

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

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

Imaginary-time interaction picture and exact Dyson identity

Split the Hamiltonian as $H_{\text{tot}} = H_0 + H_I$ with $H_0 = H_Q + H_B$. For any operator $\mathcal{O}$ define the imaginary-time interaction picture

$$\tilde{\mathcal{O}}(\tau) = e^{\tau H_0}\, \mathcal{O}\, e^{-\tau H_0}, \qquad \tau \in [0, \beta]. \tag{7}$$

The exact operator identity

$$e^{-\beta(H_0+H_I)} = e^{-\beta H_0}\, \mathcal{T}_\tau \times \exp\left(- \int_0^\beta d\tau\, \tilde{H}_I(\tau) \right) \tag{8}$$

follows from the standard imaginary-time Dyson expansion [14, 15, 26]. Since $H_I = f \otimes B$ and H_0 is a sum of commuting system and bath Hamiltonians, $\tilde{H}_I(\tau) = \tilde{f}(\tau) \otimes \tilde{B}(\tau)$ with

$$\tilde{f}(\tau) = e^{\tau H_Q} f e^{-\tau H_Q}, \qquad \tilde{B}(\tau) = e^{\tau H_B} B e^{-\tau H_B}. \tag{9}$$

Gaussian bath trace and bilocal influence functional

Tracing Eq. (8) over the bath gives

$$\rho_S^{\text{unnorm}} = e^{-\beta H_Q} \left\langle \mathcal{T}_\tau \exp\left(- \int_0^\beta d\tau\, \tilde{f}(\tau) \tilde{B}(\tau) \right) \right\rangle_B . \tag{10}$$

Assume the bath is Gaussian with respect to B (all cumulants beyond second order vanish). The cumulant expansion for ordered exponentials then yields

$$\left\langle \mathcal{T}_\tau \exp\left(- \int d\tau\, \tilde{f}(\tau) \tilde{B}(\tau) \right) \right\rangle_B = \exp\left(\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int d\tau_1 \cdots d\tau_n \; C_n(\tau_1, \ldots, \tau_n) \prod_{j=1}^{n} \tilde{f}(\tau_j) \right). \tag{11}$$

where the n-point cumulant is

$$C_n(\tau_1, \ldots, \tau_n) \equiv \langle \mathcal{T}_\tau \tilde{B}(\tau_1) \cdots \tilde{B}(\tau_n) \rangle_c. \tag{12}$$

and for a Gaussian bath only the $n = 2$ term survives. This yields the exact bilocal influence functional

$$\rho_S^{\text{unnorm}} = e^{-\beta H_Q}\, \mathcal{T}_\tau \exp\left(- \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \; \tilde{f}(\tau)\, K(\tau - \tau')\, \tilde{f}(\tau') \right). \tag{13}$$

with the thermal bath kernel

$$K(\tau - \tau') \equiv \langle \mathcal{T}_\tau\, \tilde{B}(\tau) \tilde{B}(\tau') \rangle_B, \qquad \langle \cdot \rangle_B \equiv \mathrm{Tr}_B(\cdot\, \rho_B), \qquad \rho_B = Z_B^{-1} e^{-\beta H_B}. \tag{14}$$

This bilocal form is standard for linear coupling to a harmonic bath and holds exactly under the Gaussian assumption [14, 15, 23, 24, 26].

Gaussian-field (Hubbard–Stratonovich) reformulation

The bilocal quadratic form in Eq. (13) can be linearized by a Hubbard–Stratonovich transformation, yielding an exact representation as a quenched Gaussian average

$$\rho_S^{\text{unnorm}} = e^{-\beta H_Q} \left\langle \mathcal{T}_\tau \exp\left(- \int_0^\beta d\tau\, \xi(\tau)\, \tilde{f}(\tau) \right) \right\rangle_\xi, \tag{15}$$

where $\xi(\tau)$ is a zero-mean Gaussian field with covariance $\langle \xi(\tau)\xi(\tau')\rangle = K(\tau - \tau')$. This reformulation is exact and is widely used in stochastic unravellings of imaginary-time influence functionals [21, 22, 27, 28, 30].

Time ordering and interaction-picture dynamics of the coupling operator

Although f is time independent in the Schrödinger picture, the interaction-picture operator $\tilde{f}(\tau)$ is nontrivial whenever $[H_Q, f] \neq 0$. The time ordering in Eqs. (13)–(15) acts on noncommuting operators, so one cannot replace $\tilde{f}(\tau)$ by f unless it commutes with H_Q. Explicitly,

$$\frac{d}{d\tau}\tilde{f}(\tau) = [H_Q, \tilde{f}(\tau)], \qquad \tilde{f}(0) = f, \tag{16}$$

so the ordered product $\mathcal{T}_\tau\, \tilde{f}(\tau)\tilde{f}(\tau')$ cannot be reduced to f^2 unless $[H_Q, f] = 0$. Operator differentiation and ordered exponentials are treated systematically in Refs. [31–33].

Adjoint-action expansion and kernel moments

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

$$\tilde{f}(\tau) = e^{\tau \mathrm{ad}_{H_Q}}(f) = \sum_{n=0}^{\infty} \frac{\tau^n}{n!}\, \mathrm{ad}^n_{H_Q}(f), \tag{17}$$

which follows from the exponential map for operators [31]. Substituting into the bilocal exponent of Eq. (13) yields the exact algebraic expansion

$$\int_0^\beta d\tau \int_0^\beta d\tau'\, K(\tau - \tau')\tilde{f}(\tau)\tilde{f}(\tau') = \sum_{n,m=0}^{\infty} \mu_{nm}\, \mathrm{ad}^n_{H_Q}(f)\, \mathrm{ad}^m_{H_Q}(f). \tag{18}$$

with kernel moments

$$\mu_{nm} \equiv \frac{1}{n!\, m!} \int_0^\beta d\tau \int_0^\beta d\tau'\, \tau^n (\tau')^m K(\tau - \tau'). \tag{19}$$

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

Exact closure criterion and local construction

Define the adjoint-generated subspace

$$\mathcal{A}_f = \mathrm{span}\{\mathrm{ad}^n_{H_Q}(f)\}_{n=0}^{\infty}. \tag{20}$$

Exact closure criterion. 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 BCH/Magnus series for $\log \rho_S$ closes within its enveloping algebra [32–35].

When the closure condition holds, the time-ordered exponential in Eq. (13) can be written as $\exp(\Omega)$ with Ω a finite linear combination of basis elements in the closed algebra (Magnus expansion). Combining $e^{-\beta H_Q}$ and e^{Ω} by BCH yields $\rho_S^{\text{unnorm}} = e^{-\beta H_{\text{MF}}}$ with H_{MF} in the same finite operator class. When closure fails, the Magnus/BCH series does not truncate and any finite local ansatz for H_{MF} necessarily involves 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_iO_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 [32–34].

Step 3: Kernel moments. Compute the kernel moments μ_{nm} from Eq. (19) using the bath correlation function $K(\tau - \tau')$. For harmonic baths, K is determined by the spectral density and temperature [15, 23].

Step 4: Construct H_{MF}. With the basis and moments in hand, assemble the bilocal exponent via Eq. (18), 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 $H(\tau)$,

$$\rho(\tau) \equiv \mathcal{T}_\tau \exp\left(-\int_0^\tau d\tau'\, H(\tau')\right), \quad \rho(0) = \mathbb{I}. \tag{21}$$

Standard differentiation identities for ordered exponentials imply

$$-\partial_\tau \rho(\tau) = H(\tau)\rho(\tau), \tag{22}$$

with the ordering built into $\rho(\tau)$; see, e.g., Refs. [31–33] for operator calculus and time-ordered exponentials.

In the present context one takes

$$H(\tau) = H_Q + \xi(\tau) f, \tag{23}$$

where the Gaussian field satisfies

$$\langle \xi(\tau)\xi(\tau')\rangle = K(\tau - \tau'). \tag{24}$$

The reduced equilibrium operator can be written as

$$\rho_S^{\mathrm{unnorm}} = e^{-\beta H_Q} \langle \rho(\beta)\rangle_\xi\,, \tag{25}$$

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

To connect Eq. (25) 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, 26].

Kernel Symmetry and Moment Relations

The bath kernel appearing in the bilocal influence functional is

$$K(\tau - \tau') = \mathrm{Tr}_B\left[\mathcal{T}_\tau \tilde{B}(\tau)\tilde{B}(\tau')\rho_B\right], \quad \rho_B = \frac{e^{-\beta H_B}}{Z_B}. \tag{26}$$

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

$$K(\tau - \tau') = K(\tau' - \tau), \qquad \mu_{nm} = \mu_{mn}, \tag{27}$$

where μ_{nm} are the kernel moments defined in Eq. (19). 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, 23, 24] 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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