Hamiltonian of Mean Force Beyond the Commuting Gaussian Benchmark

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We study the operator representability problem for the Hamiltonian of mean force (HMF) in Gaussian linearly coupled environments beyond the commuting limit. Building on the quenched-density construction, we derive an exact imaginary-time reformulation in which bath statistics enter as scalar kernel moments while operator growth is generated by the adjoint chain $\{\mathrm{ad}^n_{H_Q}(f)\}_{n\geq 0}$. This yields a structural criterion: a finite closed-form HMF exists only when the adjoint-generated operator algebra closes inside the target ansatz. We then instantiate the criterion in a Pauli-closed qubit model and obtain an explicit closed-form mean-force Hamiltonian with temperature- and bath-dependence carried by mode-resolved kernel coefficients. The manuscript is framed as the noncommuting Gaussian follow-up to the commuting benchmark analysis of arXiv:2602.13146 and sets up the non-Gaussian extension program.

INTRODUCTION

This manuscript is a direct follow-up to Ref. [1] (arXiv:2602.13146). That paper established the quenched-density representation and delivered an exact benchmark in the commuting Gaussian sector. The present paper starts from that benchmark and addresses the next step: how the Hamiltonian of mean force is organised once the coupling operator does *not* commute with the bare system Hamiltonian.

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,

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

$$e^{-\beta H_{\mathrm{MF}}(\beta)} \propto \frac{\mathrm{Tr}_X e^{-\beta H_{\mathrm{tot}}}}{Z_X(\beta)}, \quad Z_X(\beta) = \mathrm{Tr}_X e^{-\beta H_X}. \tag{2}$$

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 [2–5].

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[2, 5, 6]. 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 [4, 7]. Related subensemble approaches explicitly treat the subsystem thermodynamics as inherited from a global canonical ensemble, making the effective reduced generator central to the formalism[8]. 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[9, 10]. The strong-coupling literature consequently treats the mean-force Gibbs state as a distinct equilibrium object, with operational ramifications for heat and energy definitions[11, 12].

The HMF literature itself is broad but structured. Canonical definitions and thermodynamic identities are developed in strong-coupling thermodynamics and fluctuation-relation work[2, 3, 5, 6]. A comprehensive review consolidates the "static" mean-force Gibbs perspective with the "dynamical" return-to-equilibrium perspective in open quantum systems [4]. Operational questions such as measurability and thermodynamic consistency at strong coupling have also been pursued[12, 13].

Exact or controlled evaluations exist in special cases. For commuting (QND) interactions, the operator algebra closes trivially and the HMF can be written explicitly[14]. Quadratic/Gaussian models (e.g., damped harmonic oscillators) are solvable because Gaussianity is preserved, leading to closed operator forms[15–17]. Finite-dimensional closures such as spin-boson or single-qubit models provide additional controlled benchmarks[18]. 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[19]. Recent work generalizes the HMF framework to finite baths by introducing a pair of quantum Hamiltonians of mean force that incorporate bath feedback[20], and structural studies further analyze the operator content of the HMF in extended settings[21].

Outside solvable models, most approaches are perturbative or numerical. Weak-coupling/high-temperature expansions yield controlled but limited series[19]. Imaginary-time path-integral methods, stochastic representations, and hierarchical-equations techniques can compute $\bar{\rho}_Q(\beta)$ directly but typically do not provide a compact operator form for $H_{\rm MF}$[22–26]. Stochastic Liouville and partition-free approaches provide complementary numerical access to open-system equilibration without yielding closed-form HMFs [27, 28]. 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[15, 16, 29]. 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[30–32]. Related path-integral derivations of quantum Langevin dynamics make explicit the noise and dissipation structure inherited from the bath[33, 34]. 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 $\bar{\rho}_Q(\beta)$ numerically and analyzes its properties, but a general structural criterion is still lacking [19–21].

Relative to Ref. [1], the present manuscript has a narrower but deeper scope. We retain the exact Gaussian influence-functional and quenched-field identities, then use adjoint-action and Magnus/BCH organisation to study representability in the noncommuting sector. The central result is an explicit closure criterion: a finite closed-form HMF exists only when the operator algebra generated by repeated adjoint action of H_Q on the coupling operators closes inside the target ansatz. We then instantiate this criterion in a Pauli-closed qubit example, where all bath dependence is reduced to scalar kernel moments and the mean-force Hamiltonian is written in exact closed form.

QUENCHED REPRESENTATION AND INFLUENCE FUNCTIONAL

We begin by recapitulating the quenched representation introduced in Ref. [1]. To proceed directly from Sec. , we explicit the composite model. We denote the bare system Hamiltonian by H_Q and write

$$H_{\rm tot} = H_Q + H_X + H_{\rm int}, \tag{3}$$

where H_X is the bath Hamiltonian. We assume a factorizable interaction

$$H_{\rm int} = f \otimes B, \tag{4}$$

where f acts on the system and B is a bath operator. We can define the reduced equilibrium operator (up to normalisation) by $\bar{\rho}_Q(\beta) \equiv {\rm Tr}_X e^{-\beta H_{\rm tot}}$. As shown in Ref. [1], this can be represented as a *quenched density*. This is an average over a stochastic propagator, given by:

$$\bar{\rho}_Q(\beta) = \mathbb{E}_\xi\left[U_\xi(\beta)\right], \tag{5}$$

$$U_\xi(\beta) \equiv \mathcal{T}_\tau \exp\left[-\int_0^\beta d\tau \left(H_Q + \xi(\tau) f\right)\right], \tag{6}$$

where $\xi(\tau)$ is a stochastic process whose statistics encode the bath correlations, and $\mathcal{T}_\tau$ denotes time-ordering in imaginary time. Regardless of the precise form of bath and coupling, the reduced density must always be describable in this form.

This result can be understood intuitively by first observing that since the environment influence can only enter through the system coupling f, its influence can be captured by attaching a τ-dependent driving field to f [35, 36]. If this were a single deterministic field however, it would correspond to the bath exerting the *same* back-action history for every microscopic bath configuration. But ${\rm Tr}_X$ averages over many bath microstates in the thermal ensemble, and hence over many back-action histories. In this sense the partial trace is necessarily an average over histories in imaginary time, and the quenched representation simply makes this averaging explicit. For each realisation $\xi(\tau)$ the system evolves under an imaginary-time Hamiltonian $H_Q+\xi(\tau)f$; the bath is then recovered by averaging over $\xi(\tau)$ with a law chosen to reproduce the bath-induced correlations. In this sense $\xi(\tau)$ is not a physical external control field but an efficient parametrisation of the bath history $B(\tau)$ as seen through the coupling channel.

We may understand what formal properties are demanded of ξ by considering the influence functional it is required to match. Working in imaginary time, introduce the bath interaction picture:

$$B(\tau) \equiv e^{\tau H_X} B e^{-\tau H_X}, \qquad \tau \in [0, \beta], \tag{7}$$

and define the bath thermal state $\rho_X \equiv e^{-\beta H_X}/Z_X$. For an arbitrary c-number source $j(\tau)$ coupled linearly to

$B(\tau)$, the bath generates a (time-ordered) functional

$$\mathcal{Z}_X[j] \equiv \mathrm{Tr}_X \left[\mathcal{T}_\tau \exp\left(-\int_0^\beta d\tau\, j(\tau)\, B(\tau) \right) \rho_X \right]. \tag{8}$$

Here $j(\tau)$ is introduced as an external c-number source used to generate ordered bath correlators by functional differentiation. More generally, $j(\tau)$ may be any object commuting with the bath algebra (e.g. a system operator tensored with $\mathbb{I}_X$). In the influence-functional derivation it is ultimately supplied by the system history, which becomes a c-number function in the path-integral representation. In the influence-functional approach, tracing out the bath produces precisely such a functional, evaluated on the system history through the coupling channel.

From this, the bath contribution to the effective Euclidean action can be written as [15, 16, 29]

$$\mathcal{F}[f] \equiv \mathcal{Z}_X[f], \qquad \Phi[f] \equiv \log \mathcal{F}[f]. \tag{9}$$

A key structural fact is that $\Phi[f] = \log \mathcal{F}[f]$ is the *cumulant generating functional* of the bath operator $B(\tau)$ with respect to the thermal state. Concretely, the generalised (time-ordered) cumulant theorem implies the connected expansion [37, 38]

$$\begin{aligned}\Phi[f] = \sum_{n\geq 1} \frac{(-1)^n}{n!} \int_0^\beta & d\tau_1 \cdots d\tau_n \\ & \times K^{(n)}(\tau_1, \ldots, \tau_n)\, f(\tau_1) \cdots f(\tau_n),\end{aligned} \tag{10}$$

where the kernels $K^{(n)}$ are the *connected* (cumulant) bath correlators, defined via [39]

$$K^{(n)}(\tau_1, \ldots, \tau_n) \equiv \left\langle \mathcal{T}_\tau B(\tau_1) \cdots B(\tau_n) \right\rangle_c. \tag{11}$$

The explicit connection back to Eq. (8) is given via its functional differentiation:

$$\left\langle \mathcal{T}_\tau B(\tau_1) \cdots B(\tau_n) \right\rangle_c = (-1)^n \left. \frac{\delta^n \log \mathcal{Z}_X[j]}{\delta j(\tau_1) \cdots \delta j(\tau_n)} \right|_{j=0}. \tag{12}$$

The bath influence is then completely characterised by the hierarchy $\{K^{(n)}\}_{n\geq 1}$.

To connect the influence functional back to the quenched density, we use the fact that the bath influence depends on the system history only through the linear functional $\int_0^\beta d\tau\, f(\tau) B(\tau)$. One may therefore represent $\mathcal{F}[f]$ as the (generalised) characteristic functional of an auxiliary field $\xi(\tau)$ [30–32]:

$$\mathcal{F}[f] = \mathbb{E}_\xi \left[\exp\left(-\int_0^\beta d\tau\, \xi(\tau)\, f(\tau) \right) \right], \tag{13}$$

where $\mathbb{E}_\xi[\cdot]$ denotes averaging with respect to a (possibly complex) measure on ξ-histories chosen such that (13) holds.

Since $\xi(\tau)$ is a commuting c-number field, its n-point moments are symmetric under permutations of the time arguments. The influence kernels $K^{(n)}$ fix the *cumulants* of ξ via

$$\left\langle \xi(\tau_1) \cdots \xi(\tau_n) \right\rangle_c = K^{(n)}(\tau_1, \ldots, \tau_n). \tag{14}$$

Consequently, the ordinary correlation functions of the noise are obtained from $\{K^{(m)}\}$ by the standard moment-cumulant relations:

$$\left\langle \xi(\tau_1) \cdots \xi(\tau_n) \right\rangle = \sum_{\pi \in \mathcal{P}_n} \prod_{C \in \pi} K^{(|C|)}\big(\{\tau_i\}_{i\in C}\big), \tag{15}$$

where $\mathcal{P}_n$ denotes the set of all partitions of the index set $\{1, \ldots, n\}$, and C are the disjoint blocks of a given partition $\pi \in \mathcal{P}_n$. After shifting the mean so that $K^{(1)}(\tau) = \langle \xi(\tau) \rangle = 0$, one has (for example)

$$\left\langle \xi(\tau_1)\xi(\tau_2) \right\rangle = K^{(2)}(\tau_1, \tau_2), \tag{16}$$

$$\left\langle \xi(\tau_1)\xi(\tau_2)\xi(\tau_3) \right\rangle = K^{(3)}(\tau_1, \tau_2, \tau_3), \tag{17}$$

$$\begin{aligned}\big\langle \xi(\tau_1)\xi(\tau_2)&\xi(\tau_3)\xi(\tau_4) \big\rangle \\ &= K^{(4)}(\tau_1, \tau_2, \tau_3, \tau_4) \\ &\quad + K^{(2)}(\tau_1, \tau_2) K^{(2)}(\tau_3, \tau_4) \\ &\quad + K^{(2)}(\tau_1, \tau_3) K^{(2)}(\tau_2, \tau_4) \\ &\quad + K^{(2)}(\tau_1, \tau_4) K^{(2)}(\tau_2, \tau_3).\end{aligned} \tag{18}$$

QUENCHED DENSITY AND THE HAMILTONIAN OF MEAN FORCE

The Hamiltonian of mean force is, by definition, the operator whose Gibbs form reproduces the system's reduced equilibrium state. Equivalently, it is the *operator logarithm* of the unnormalised reduced equilibrium operator

$$\bar{\rho}_Q(\beta) \equiv \mathrm{Tr}_X e^{-\beta H_{\mathrm{tot}}}, \qquad H_{\mathrm{MF}}(\beta) \;\equiv\; -\frac{1}{\beta} \log \bar{\rho}_Q(\beta), \tag{19}$$

defined up to an additive multiple of the identity (fixed only when normalising the state).

The quenched representation in Eq. (5) supplies an exact stochastic parametrisation of the unnormalised mean-force Gibbs operator $\bar{\rho}_Q(\beta)$ by making the bath trace an explicit average over imaginary-time back-action histories. Combining Eq. (5) with Eq. (19) yields

$$H_{\mathrm{MF}}(\beta) = -\frac{1}{\beta} \log \mathbb{E}_\xi [U_\xi(\beta)]\,. \tag{20}$$

Thus, constructing the mean-force Hamiltonian reduces to evaluating a stochastic average and then compressing the result via an operator logarithm. The conditions for being able to perform this average exactly is the focus of the present work.

To make the handling of this problem more concrete, we shall specialise the environment to the Caldeira-Leggett model, where the bath is a collection of harmonic oscillators ($H_X = \sum_k \omega_k b_k^\dagger b_k$) and the coupling is linear in bath coordinates ($B = \sum_k c_k x_k$). None of the results that follow are essentially dependent on this choice, and a generalisation to anharmonic environments is (relatively) straightforward. In the interests of comprehensibility however, we restrict our scope to quadratic environments. In this setting, the auxiliary field $\xi(\tau)$ becomes a stationary zero-mean Gaussian process completely characterized by its covariance

$$\mathbb{E}_\xi[\xi(\tau)\xi(\tau')] = K(\tau - \tau'). \tag{21}$$

The kernel $K(\tau)$ is determined by the bath spectral density $J(\omega) = \frac{\pi}{2}\sum_k \frac{c_k^2}{m_k\omega_k}\delta(\omega - \omega_k)$ via the relation [40]

$$K(\tau) = \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\,\frac{\cosh\big(\omega(\beta/2 - |\tau|)\big)}{\sinh(\beta\omega/2)}. \tag{22}$$

A key property of this kernel is its integrated strength. Integrating Eq. (22) yields

$$\begin{aligned}\int_0^\beta d\tau\, K(\tau) &= \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\int_0^\beta d\tau\,\frac{\cosh\big(\omega(\beta/2 - |\tau|)\big)}{\sinh(\beta\omega/2)}\\ &= \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\,\frac{2}{\omega}\\ &= 2\lambda,\end{aligned} \tag{23}$$

where λ is the explicit reorganisation energy. Consequently, the total variance of the integrated noise field $\Xi = \int_0^\beta d\tau\,\xi(\tau)$ grows linearly with inverse temperature:

$$\mathbb{E}_\xi[\Xi^2] = \int_0^\beta d\tau\int_0^\beta d\tau'\, K(\tau - \tau') = 2\beta\lambda. \tag{24}$$

In the case that the system and its coupling commute, $[H_Q, f] = 0$ and f is τ-independent in imaginary time. In this instance time ordering drops out, and the average is given by [1]:

$$\bar{\rho}_Q(\beta) = \exp\left[-\beta\left(H_Q - \frac{\kappa_0(\beta)}{2}f^2\right)\right], \tag{25}$$

which in turn yields

$$H_{\mathrm{MF}}(\beta) = H_Q - \frac{\kappa_0(\beta)}{2}f^2 + \frac{1}{\beta}\log Z_X(\beta)\,\mathbb{I}. \tag{26}$$

Notably this correction to $H_{\mathrm{MF}}(\beta)$ is entirely *classical* [1]. This is hardly surprising, but emphasises that truly quantum effects *always* stem from non-commutativity. Truly quantum thermodynamic effects are therefore only present when $[H_Q, f] \neq 0$. In this case however, the noise enters through a noncommuting operator inside $\mathcal{T}_\tau$, rendering the question of averaging highly non-trivial. In the next section, we attack this problem directly, deriving conditions under which $H_{\mathrm{MF}}(\beta)$ possesses a closed form.

CLOSURE OF THE HAMILTONIAN OF MEAN FORCE

The obstruction to writing $H_{\mathrm{MF}}(\beta)$ in a compact operator form is not the existence of the mean-force object (it is defined by a logarithm), but the *representability* of that logarithm inside a restricted operator family (few-body, local, Pauli strings, etc.). In the harmonic case this representability question reduces to a precise closure problem. To show this, we first write the quenched propagator in the imaginary-time interaction picture with respect to H_Q:

$$\begin{aligned}U_\xi(\beta) &= e^{-\beta H_Q}W_\xi(\beta),\\ W_\xi(\beta) &\equiv \mathcal{T}_\tau \exp\left[-\int_0^\beta d\tau\,\xi(\tau)\,\tilde{f}(\tau)\right],\end{aligned} \tag{27}$$

where $\tilde{f}(\tau) \equiv e^{\tau H_Q} f e^{-\tau H_Q}$.

Because the noise is classical Gaussian with zero mean, the average of the time-ordered exponential resums exactly in terms of the second cumulant,

$$\langle W_\xi(\beta)\rangle_\xi = \exp\left[\frac{1}{2}\int_0^\beta d\tau\int_0^\beta d\tau'\, K(\tau-\tau')\,\mathcal{T}_\tau\big(\tilde{f}(\tau)\tilde{f}(\tau')\big)\right]. \tag{28}$$

Using the kernel symmetry $K(\tau - \tau') = K(\tau' - \tau)$ on $[0, \beta]$ the time-ordering on the square domain reduces to a single ordered triangle with an *anticommutator*, and the influence exponent may be written as as the manifestly Hermitian operator

$$\bar{W}(\beta) = \exp\big(\Delta(\beta)\big), \qquad \bar{\rho}_Q(\beta) = \langle U_\xi(\beta)\rangle_\xi = e^{-\beta H_Q}\, e^{\Delta(\beta)}. \tag{29}$$

with the exponent $\Delta(\beta)$ given by

$$\Delta(\beta) \equiv \int_0^\beta d\tau\int_0^\tau d\tau'\, K(\tau - \tau')\,\frac{1}{2}\{\tilde{f}(\tau), \tilde{f}(\tau')\}. \tag{30}$$

To progress, we introduce the adjoint chain generated by H_Q acting on the coupling,

$$f_n \equiv \mathrm{ad}^n_{H_Q}(f), \qquad \mathrm{ad}_{H_Q}(A) \equiv [H_Q, A], \tag{31}$$

so that the interaction-picture operator has the exact series

$$\tilde{f}(\tau) = e^{\tau H_Q} f e^{-\tau H_Q} = \sum_{n\geq 0}\frac{\tau^n}{n!}\, f_n. \tag{32}$$

Substituting (32) into (30) yields

$$\Delta(\beta) = \sum_{n,m\geq 0} C^{>}_{nm}(\beta)\,\frac{1}{2}\{f_n, f_m\}.. \tag{33}$$

with the *kernel-moment matrix*

$$C^{>}_{nm}(\beta) \equiv \int_0^\beta d\tau\int_0^\tau d\tau'\, K(\tau - \tau')\,\frac{\tau^n}{n!}\,\frac{\tau'^m}{m!}. \tag{34}$$

It is convenient to symmetrise this expression with $C_n m(\beta) = (C^{>}_{nm}(\beta) + C^{<}_{nm}(\beta))/2$, where $C^{<}_{nm}(\beta) = (C^{>}_{mn}(\beta))$. This restores a square integration definition,

$$C_{nm}(\beta) = \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\, K(\tau-\tau')\,\frac{\tau^n}{n!}\,\frac{\tau'^m}{m!}, \tag{35}$$

such that the exponent becomes

$$\Delta(\beta) = \sum_{n,m\geq 0} C_{nm}(\beta) f_n f_m. \tag{36}$$

Thus all bath/temperature dependence enters $\Delta(\beta)$ only through the scalar moments $C_{nm}(\beta)$, while all operator structure is carried by the adjoint chain $\{f_n\}$. The final step is to re-express the averaged propagator in a *single* exponential. Using (29) we write

$$\bar{\rho}_Q(\beta) = e^{-\beta H_Q}\, e^{\Delta(\beta)} \equiv e^{-\beta H_{\mathrm{MF}}(\beta)}, \tag{37}$$

where the mean-force Hamiltonian satisfies

$$-\beta H_{\mathrm{MF}}(\beta) = \log\Big(e^{-\beta H_Q} e^{\Delta(\beta)}\Big). \tag{38}$$

Let $A \equiv -\beta H_Q$ and $B \equiv \Delta(\beta)$. The Baker–Campbell–Hausdorff (BCH) series gives

$$\begin{aligned}\log(e^A e^B) &= A + B + \frac{1}{2}[A,B]\\ &\quad + \frac{1}{12}[A,[A,B]] + \frac{1}{12}[B,[B,A]] + \cdots.\end{aligned} \tag{39}$$

Dividing by $-\beta$ and using $A = -\beta H_Q$ yields the expansion

$$\begin{aligned}H_{\mathrm{MF}}(\beta) = H_Q &- \frac{1}{\beta}\Delta(\beta) + \frac{1}{2}[H_Q,\Delta(\beta)]\\ &- \frac{\beta}{12}[H_Q,[H_Q,\Delta(\beta)]]\\ &+ \frac{1}{12}[\Delta(\beta),[\Delta(\beta),H_Q]] + \cdots.\end{aligned} \tag{40}$$

This expansion is our main result - an exact expression for the mean-force Hamiltonian in terms of the exact influence operator. Expressed in this way, the closure content of $H_{\mathrm{MF}}(\beta)$ is transparent: all terms are built from repeated commutators with H_Q acting on Δ, together with higher BCH terms involving commutators among those objects.

To see the explicit generator, introduce the adjoint superoperator $\mathrm{ad}_{H_Q}(\cdot) \equiv [H_Q,\cdot]$. Then (40) becomes

$$\begin{aligned}H_{\mathrm{MF}}(\beta) = H_Q &- \frac{1}{\beta}\Delta + \frac{1}{2}\,\mathrm{ad}_{H_Q}\Delta\\ &- \frac{\beta}{12}\,\mathrm{ad}^2_{H_Q}\Delta + \frac{1}{12}\,[\Delta,\mathrm{ad}_{H_Q}\Delta] + \cdots.\end{aligned} \tag{41}$$

Finally, because $\Delta(\beta)$ is quadratic in the adjoint chain, each commutator with H_Q simply shifts indices:

$$\mathrm{ad}_{H_Q}(f_n f_m) = [H_Q, f_n f_m] = f_{n+1} f_m + f_n f_{m+1}. \tag{42}$$

Hence the first commutator term takes the explicit form

$$[H_Q,\Delta(\beta)] = \frac{1}{2}\sum_{n,m\geq 0} C_{nm}(\beta)\,\big(f_{n+1}f_m + f_n f_{m+1}\big), \tag{43}$$

and higher $\mathrm{ad}^k_{H_Q}\Delta$ generate the same family of products $f_a f_b$ with shifted indices. The remaining BCH terms (e.g. $[\Delta,\mathrm{ad}_{H_Q}\Delta]$) introduce commutators among these quadratic elements, and are the sole source of additional operator growth beyond the quadratic span. The only remaining question is whether the operator family generated by (41) can be brought to a closed form.

The preceding identities imply that the entire BCH commutator tower *linear* in Δ remains within the quadratic span $\mathrm{span}\{f_n f_m\}$. Terms to this order explicitly admit a closed resummation. Let $A \equiv -\beta H_Q$ and $B \equiv \Delta(\beta)$. Then the BCH logarithm satisfies the standard linear-in-B identity

$$\begin{aligned}\log\big(e^A e^B\big) &= A + \Phi\big(\mathrm{ad}_A\big)\,B + O(B^2),\\ \Phi(x) &\equiv \frac{x}{1-e^{-x}}.\end{aligned} \tag{44}$$

Substituting $A = -\beta H_Q$ and dividing by $-\beta$ gives the mean-force Hamiltonian to first order in Δ:

$$H_{\mathrm{MF}}(\beta) = H_Q - \frac{1}{\beta}\,\Phi\big(\beta\,\mathrm{ad}_{H_Q}\big)\,\Delta(\beta) + O(\Delta^2). \tag{45}$$

Expanding Φ yields the explicit commutator series with Bernoulli numbers B_k,

$$\begin{aligned}H_{\mathrm{MF}}(\beta) &= H_Q - \frac{1}{\beta}\sum_{k\geq 0}\frac{B_k}{k!}(-\beta)^k\,\mathrm{ad}^k_{H_Q}\Delta(\beta) + O(\Delta^2),\\ \Phi(x) &= \sum_{k\geq 0}\frac{B_k}{k!}(-x)^k.\end{aligned} \tag{46}$$

Using (42) repeatedly, the iterated commutators admit the closed binomial form

$$\mathrm{ad}^k_{H_Q}(f_n f_m) = \sum_{j=0}^{k}\binom{k}{j} f_{n+j}\, f_{m+k-j}, \tag{47}$$

so every term in (46) is explicitly a linear combination of products $f_a f_b$ with scalar coefficients determined solely by $C_{nm}(\beta)$ and universal combinatorics. Because of this, we may bring the first order contribution into a particularly compact form by introducing the discrete shift operator D. This will act on the moment matrix C as

$$\begin{aligned}(\mathsf{D}C)_{ab} &\equiv C_{a-1,b} + C_{a,b-1},\\ C_{rs} &\equiv 0 \quad \text{if any index is negative.}\end{aligned} \tag{48}$$

Then (42) implies, after reindexing,

$$\mathrm{ad}_{H_Q}\Delta(\beta) = \frac{1}{2}\sum_{a,b\geq 0}(\mathsf{D}C(\beta))_{ab}\, f_a f_b, \tag{49}$$

and by iteration,

$$\mathrm{ad}_{H_Q}^k \Delta(\beta) = \frac{1}{2} \sum_{a,b\geq 0} (\mathsf{D}^k C(\beta))_{ab}\, f_a f_b. \tag{50}$$

Equivalently, $(\mathsf{D}^k C)_{ab} = \sum_{j=0}^k \binom{k}{j} C_{a-j,\, b-(k-j)}$, which is the binomial index-shift structure implied by (47). From this we obtain the following form for $H_{\mathrm{MF}}(\beta)$ to linear order in Δ:

$$H_{\mathrm{MF}}(\beta) = H_Q - \frac{1}{2\beta} \sum_{a,b\geq 0} \widetilde{C}_{ab}(\beta)\, f_a f_b \;+\; O(\Delta^2), \tag{51}$$

where the *renormalised moment matrix* $\widetilde{C}(\beta)$ is the universal transform

$$\widetilde{C}(\beta) \equiv \Phi\big(\beta\, \mathsf{D}\big)\, C(\beta) = \sum_{k\geq 0} \frac{B_k}{k!} (-\beta)^k\, \mathsf{D}^k C(\beta). \tag{52}$$

Thus, to linear order in the influence operator, the mean-force Hamiltonian is *exactly* a quadratic form in the products $f_a f_b$, with all bath/temperature dependence entering only through the scalar matrix $\widetilde{C}_{ab}(\beta)$. Any operator growth beyond the quadratic span is confined to the nonlinear BCH sector $O(\Delta^2)$ (e.g. $[\Delta, \mathrm{ad}_{H_Q}\Delta]$). While these terms are more difficult to handle as they involve commutators of quadratic forms, they nevertheless admit a precise series expansion via the full BCH formula (39).

With this form in hand, we can now state a theorem for the representability of $H_{\mathrm{MF}}(\beta)$ in a given operator family $\mathcal{A}$ as a *closure criterion.*

Theorem: Finite representability of mean force

Fix a target operator family $\mathcal{A}$ (e.g. k-local Pauli strings, a Lie algebra plus identity, or a finite-dimensional associative operator algebra) in which we seek to represent $H_{\mathrm{MF}}(\beta)$. The Gaussian construction above allows us to formulate the exact criteria for representability as a closure theorem. In a physical sense, these conditions determine whether a valid *local generator* can be defined for the system at all; failure of closure implies that the effective Hamiltonian is fundamentally non-local with respect to the algebra $\mathcal{A}$.

Theorem (Closure of the Mean Force). *Let $\mathcal{A}$ be a target operator space containing the bare system Hamiltonian H_Q. The Hamiltonian of Mean Force $H_{\mathrm{MF}}(\beta)$ admits a finite representation within $\mathcal{A}$ if and only if the following three closure conditions are satisfied:*

(C1) Adjoint Closure (No linear operator growth). The subspace generated by repeated commutators of the coupling f with H_Q must remain inside $\mathcal{A}$:

$$\begin{gathered} f \in \mathcal{A}, \qquad \mathrm{ad}_{H_Q}(\mathcal{A}) \subseteq \mathcal{A}, \\ \text{equivalently} \quad \mathrm{span}\{f_n\}_{n\geq 0} \subseteq \mathcal{A}. \end{gathered} \tag{53}$$

(C2) Quadratic Closure (No growth in the Gaussian sector). Because the exact influence operator $\Delta(\beta)$ is quadratic in the adjoint chain, the quadratic span generated by $\{f_n\}$ must also lie in $\mathcal{A}$:

$$f_n f_m \in \mathcal{A} \quad \text{for all indices that contribute in } \Delta(\beta), \tag{54}$$

so that $\Delta(\beta) \in \mathcal{A}$. A sufficient (and common) condition is that $\mathcal{A}$ is an associative algebra containing the identity and closed under multiplication.

(C3) BCH Closure (No growth from commutators among quadratic elements). To ensure that the *full* BCH logarithm $\log(e^{-\beta H_Q} e^{\Delta})$ remains in $\mathcal{A}$, the commutators generated among the quadratic elements must also close in $\mathcal{A}$; in particular

$$[\Delta(\beta),\, \mathrm{ad}_{H_Q}^k \Delta(\beta)] \in \mathcal{A} \qquad \text{for all } k \geq 0, \tag{55}$$

and similarly for the higher nested commutators appearing in the BCH series. A sufficient (and common) condition is again that $\mathcal{A}$ is a finite-dimensional associative algebra (or a Lie algebra containing Δ and closed under commutators), in which case all BCH commutators remain in $\mathcal{A}$ by construction.

Consequence (closed-form mean-force Hamiltonian). If (C1)–(C3) hold, then $\Delta(\beta) \in \mathcal{A}$ and all BCH commutators generated by (56) remain in $\mathcal{A}$. Since $H_Q \in \mathcal{A}$ by assumption, it follows that

$$\begin{aligned} \bar{\rho}_Q(\beta) &= e^{-\beta H_{\mathrm{MF}}(\beta)}, \\ -\beta H_{\mathrm{MF}}(\beta) &= \log\Big(e^{-\beta H_Q} e^{\Delta(\beta)}\Big), \end{aligned} \tag{56}$$

defines an $H_{\mathrm{MF}}(\beta) \in \mathcal{A}$ and hence a closed-form representation of $H_{\mathrm{MF}}(\beta)$ (up to the usual additive scalar fixed by Z_X). If either (C1) fails (adjoint-chain growth) or (C2)–(C3) fail (growth in the quadratic/BCH sector), then $\Delta(\beta)$ and/or the BCH commutator tower generates operators outside $\mathcal{A}$; any representation within $\mathcal{A}$ is necessarily truncated or projected.

This statement leads to an important corollary. For continuous variable systems $H_Q = p^2/2m + V(x)$, if the potential $V(x)$ is a polynomial of degree greater than 2, the adjoint chain $\{f_n\}$ generally does not close in any finite-dimensional Lie algebra; instead, it generates the full universal enveloping algebra. Consequently, no finite representation of the mean force exists. This obstruction shares a common origin with the ordering ambiguity in quantisation (Groenewold-Van Hove theorem): the failure to close the operator algebra corresponds to the impossibility of consistently mapping the quantum evolution of non-quadratic potentials to a finite classical phase space flow. This result extends the impossibility: for such potentials, there is not even a *local operator* which can describe the equilibrium state exactly.

From a practical standpoint, the closure of $\mathcal{A}$ is not necessary for an arbitrarily accurate approximation of

$H_{\mathrm{MF}}(\beta)$, as the BCH logarithm $\log(e^{-\beta H_Q}e^{\Delta})$ still yields a controlled expansion. The operator content is generated by the adjoint chain and its quadratic products, while all bath dependence remains scalar through $C_{nm}(\beta)$. One may therefore truncate (in commutator depth, locality class, or operator weight) without introducing any approximation on the bath side.

This algebraic perspective offers a unifying view of strong-coupling approximations. Numerical schemes such as the polaron transformation [40], hierarchical equations of motion [25], and chain-mapping/DMRG techniques can be understood as distinct choices of the target operator family $\mathcal{A}$. The polaron frame corresponds to dressing $\mathcal{A}$ with coherent displacements; HEOM truncates the memory depth of the influence functional (dual to the operator degree in the adjoint chain), and chain mappings truncate the spatial extent of the harmonic bath. The 'closure' problem is thus equivalent to identifying a low-dimensional subalgebra that approximately contains the logarithm of the quenched propagator.

Exact mean-force Hamiltonian for the transverse-coupling spin-boson model

We now turn to applying the results developed in the previous section. A particularly instructive example concerns spins, as the su(2) algebra is sufficiently simple at to permit an exact analytic solution. We demonstrate this by applying it to a transverse-coupling spin-boson model. Following Ref. [19], let

$$H_Q = \frac{\omega_q}{2}\sigma_z, \qquad f = \cos\theta\,\sigma_z - \sin\theta\,\sigma_x, \tag{57}$$

with $c \equiv \cos\theta$, $s \equiv \sin\theta$ throughout. The coupling mixes a commuting part $c\sigma_z$ with a transverse part $-s\sigma_x$.

Using $[H_Q, \sigma_x] = i\omega_q\sigma_y$ and $[H_Q, \sigma_y] = -i\omega_q\sigma_x$, the σ_z component of f is annihilated by ad_{H_Q} while the transverse part precesses. A direct induction gives

$$f_n \equiv \mathrm{ad}^n_{H_Q}(f) = \begin{cases} c\,\sigma_z - s\,\sigma_x & n = 0, \\ -s\,\omega_q^n\,\sigma_x & n \geq 1,\ n \text{ even}, \\ -is\,\omega_q^n\,\sigma_y & n \geq 1,\ n \text{ odd}. \end{cases} \tag{58}$$

The adjoint chain therefore closes on $\mathrm{span}\{\sigma_x, \sigma_y, \sigma_z\}$, satisfying condition (C1) We now evaluate each sector of products $f_n f_m$ using the Pauli identities $\sigma_j^2 = \mathbb{I}$ and $\sigma_j\sigma_k = \delta_{jk}\mathbb{I} + i\epsilon_{jkl}\sigma_l$. Dropping $\mathbb{I}$ terms throughout (they contribute only to the normalisation), the non-trivial contributions to each Pauli component can be summarized by cases. For indices n, m yielding non-vanishing terms, we find:

$$f_n f_m \cong \begin{cases} is^2\omega_q^{n+m}\sigma_z & n \in 2\mathbb{N}, m \in 2\mathbb{N}-1, \\ -is^2\omega_q^{n+m}\sigma_z & n \in 2\mathbb{N}-1, m \in 2\mathbb{N}, \\ cs\omega_q^m\sigma_x - s^2\omega_q^m\sigma_z & n = 0, m \in 2\mathbb{N}-1, \\ cs\omega_q^n\sigma_x + s^2\omega_q^n\sigma_z & n \in 2\mathbb{N}-1, m = 0. \end{cases} \tag{59}$$

Terms generating σ_y are omitted as they vanish by the symmetry $C_{nm} = C_{mn}$. The σ_z contributions from the $n, m \geq 1$ sector also vanish by this symmetry, as the cases n even, m odd and n odd, m even enter with opposite signs. The only σ_z contributions then come from the $n = 0$ cross terms. This confirms condition (C2) is also satisfied.

Inserting these into Eq.(66), we now enumerate each component of Δ. For the σ_z component, we have

$$\Delta\big|_{\sigma_z} = -2s^2\sum_{m=0}^{\infty} C_{0,2m+1}\,\omega_q^{2m+1}\,\sigma_z, \tag{60}$$

where the symmetry $C_{0m} = C_{m0}$ has again been employed. Similarly for the σ_x component, we obtain

$$\Delta\big|_{\sigma_x} = 2cs\sum_{m=0}^{\infty} C_{0,2m+1}\,\omega_q^{2m+1}\,\sigma_x. \tag{61}$$

From this we find that the non-trivial operator content of $\Delta(\beta)$ is controlled by the single sum

$$\begin{aligned} &\sum_{m=0}^{\infty} C_{0,2m+1}\,\omega_q^{2m+1} \\ &\quad = \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K(\tau-\tau')\sum_{m=0}^{\infty}\frac{(\omega_q\tau')^{2m+1}}{(2m+1)!} \\ &\quad = \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K(\tau-\tau')\sinh(\omega_q\tau'), \end{aligned} \tag{62}$$

From this we may define the *effective kernel*:

$$\mathcal{K}(\beta) \equiv \int_0^\beta d\tau \int_0^\beta d\tau'\,K(\tau-\tau')\sinh(\omega_q\tau'). \tag{63}$$

Using the periodicity of the kernel $K(\tau) = K(\tau+\beta)$, the integral over the first variable τ decouples from τ':

$$\int_0^\beta d\tau\,K(\tau-\tau') = \int_{-\tau'}^{\beta-\tau'} du\,K(u) = \int_0^\beta du\,K(u). \tag{64}$$

The remaining integral over $\sinh(\omega_q\tau')$ can be performed directly. Identifying the integrated kernel strength with the reorganization energy via Eq. (23), $\int_0^\beta d\tau K(\tau) = 2\lambda$, we obtain:

$$\mathcal{K}(\beta) = 2\lambda\int_0^\beta d\tau'\sinh(\omega_q\tau') = \frac{4\lambda}{\omega_q}\sinh^2\left(\frac{\beta\omega_q}{2}\right), \tag{65}$$

which leads to the a compact final form for the influence exponent:

$$\begin{aligned}\Delta(\beta) &= \mathcal{K}(\beta)\big(cs\,\sigma_x - s^2\,\sigma_z\big)\\ &= s\,\mathcal{K}(\beta)\big(c\,\sigma_x - s\,\sigma_z\big).\end{aligned} \tag{66}$$

Amusingly, we see that the form of $\Delta(\beta)$ lies orthogonal to the original coupling $f = c\sigma_z - s\sigma_x$ in the xz-plane.

The final step is to recombine $\Delta(\beta)$ with $-\beta H_Q$ to obtain the mean-force Hamiltonian. This generically requires condition (C3), but in this case our task is simplified greatly as both $-\beta H_Q$ and $\Delta(\beta)$ are elements of $\mathfrak{su}(2)$. Thus their combined exponential is given by

$$\begin{aligned}\bar{\rho}_Q(\beta) &= e^{-\beta H_Q} e^{\Delta(\beta)}\\ &= e^{\boldsymbol{a}\cdot\boldsymbol{\sigma}} e^{\boldsymbol{b}\cdot\boldsymbol{\sigma}} = e^{\boldsymbol{\nu}\cdot\boldsymbol{\sigma}}\end{aligned} \tag{67}$$

We apply this by setting $\boldsymbol{a} = -\frac{\beta\omega_q}{2}\hat{z}$ and $\boldsymbol{b} \equiv \delta_x\hat{x} + \delta_z\hat{z}$, with $\delta_x = cs\,\mathcal{K}$ and $\delta_z = -s^2\,\mathcal{K}$ This then points in the fixed direction $c\hat{x} - s\hat{z}$ with magnitude

$$\Omega_\Delta \equiv |\boldsymbol{b}| = \sqrt{\delta_x^2 + \delta_z^2} = s\,\mathcal{K}(\beta). \tag{68}$$

The composition rule for $\boldsymbol{\nu}$ is

$$\cos|\boldsymbol{\nu}| = \cos|\boldsymbol{a}|\cos|\boldsymbol{b}| - \hat{a}\cdot\hat{b}\,\sin|\boldsymbol{a}|\sin|\boldsymbol{b}|, \tag{69}$$

$$\frac{\boldsymbol{\nu}}{|\boldsymbol{\nu}|} = \frac{1}{\sin|\boldsymbol{\nu}|}\Big[\sin|\boldsymbol{a}|\cos|\boldsymbol{b}|\,\hat{a} + \cos|\boldsymbol{a}|\sin|\boldsymbol{b}|\,\hat{b} + \sin|\boldsymbol{a}|\sin|\boldsymbol{b}|\,(\hat{a}\times\hat{b})\Big]. \tag{70}$$

With $\hat{a} = -\hat{z}$, $\hat{b} = c\hat{x} - s\hat{z}$, we have $\hat{a}\cdot\hat{b} = s$ and

$$\hat{a}\times\hat{b} = -\hat{z}\times(c\hat{x} - s\hat{z}) = -c\,\hat{y}, \tag{71}$$

so a σ_y component is generated by the noncommutativity of H_Q and Δ. Substituting $|\boldsymbol{a}| = \beta\omega_q/2$ and $|\boldsymbol{b}| = s\mathcal{K}$, (69) gives

$$\cos\Omega \equiv \cos\tfrac{\beta\omega_q}{2}\cos\Omega_\Delta + s\sin\tfrac{\beta\omega_q}{2}\sin\Omega_\Delta, \tag{72}$$

which defines $\Omega \equiv |\boldsymbol{\nu}|$. The resulting vector $\boldsymbol{\nu}$ has a nonzero y-component (70), indicating that H_{MF} contains a term $\propto \sigma_y$. However, the structure of (70) allows this to be removed by a simple frame rotation.

Specifically, the transverse part of $\boldsymbol{\nu}$ lies at an angle $-\beta\omega_q/2$ in the xy-plane. We may therefore eliminate ν_y by applying the unitary transformation $U_0 = e^{-i\frac{\beta\omega_q}{4}\sigma_z}$, which rotates the frame by an angle $\phi = \beta\omega_q/2$ about the z-axis. In this rotated frame, the mean-force Hamiltonian $H'_{\mathrm{MF}} = U_0 H_{\mathrm{MF}} U_0^\dagger$ is determined by the vector $\boldsymbol{\nu}'$ with components:

$$\nu'_x = c\,\frac{\Omega}{\sin\Omega}\sin(s\mathcal{K}), \tag{73}$$

$$\nu'_z = \frac{\Omega}{\sin\Omega}\Big[-\sin\tfrac{\beta\omega_q}{2}\cos(s\mathcal{K}) - s\cos\tfrac{\beta\omega_q}{2}\sin(s\mathcal{K})\Big]. \tag{74}$$

The mean-force Hamiltonian is thus physically equivalent to the clean form

$$H_{\mathrm{MF}}(\beta) = -\frac{1}{\beta}\boldsymbol{\nu}\cdot\boldsymbol{\sigma} = h_x(\beta)\,\sigma_x + h_z(\beta)\,\sigma_z, \tag{75}$$

where we have dropped the primes for brevity. The dependence on the bath is entirely captured by effective kernel $\mathcal{K}(\beta)$ and the mixing angle θ (via c, s).

This form allows for a direct analysis of the coupling limits. The coupling strength g enters exclusively through the reorganization energy $\lambda \propto g^2$, which in turn scales the effective kernel $\mathcal{K}(\beta) \propto g^2$.

1. **Weak Coupling ($\lambda \to 0$):** In this limit $\mathcal{K} \to 0$, implying $s\mathcal{K} \to 0$. We immediately have $\nu_x \to 0$ and $\nu_z \to -\frac{\beta\omega_q}{2}$. Thus $H_{\mathrm{MF}} \to \frac{\omega_q}{2}\sigma_z = H_Q$, recovering the bare system Hamiltonian as expected.

2. **Ultrastrong Coupling ($\lambda \to \infty$):** Here $s\mathcal{K} \propto g^2 \gg 1$. In this regime the bath term dominates the free evolution phase $\beta\omega_q$, so $\Omega \approx s\mathcal{K}$. The vector components simplify to:

$$\nu_x \approx c\,\frac{s\mathcal{K}}{\sin(s\mathcal{K})}\sin(s\mathcal{K}) = c\,s\mathcal{K}, \tag{76}$$

$$\nu_z \approx -s\,\frac{s\mathcal{K}}{\sin(s\mathcal{K})}\sin(s\mathcal{K}) = -s^2\mathcal{K}. \tag{77}$$

The mean-force Hamiltonian becomes

$$H_{\mathrm{MF}} \approx -\frac{s\mathcal{K}}{\beta}(c\sigma_x - s\sigma_z) = \frac{s\mathcal{K}}{\beta}f. \tag{78}$$

This result is physically transparent: at ultrastrong coupling, the mean-force potential is simply the system-bath coupling operator f scaled by the reorganization energy directly.

NUMERICAL VALIDATION AGAINST WEAK/ULTRASTRONG PREDICTIONS

We benchmark the qubit predictions of Ref. [19] against exact finite-bath trace-out calculations over the full coupling range, using Sec. **??** as the analytic target: the direct-kernel Gaussian weak target in Eqs. (**??**)–(**??**) and the ultrastrong projector state in Eq. (**??**). The system Hamiltonian and coupling operator are

$$H_S = \frac{\omega_q}{2}\sigma_z, \qquad X = \cos\theta\,\sigma_z - \sin\theta\,\sigma_x, \tag{79}$$

with $\omega_q = 3$ and $\theta = 0.25$. The bath is discretised from $J(\omega) = Q\tau_c\omega e^{-\tau_c\omega}$ using $N_\omega = 3$ modes over $[0.5, 8.0]$, per-mode cutoff $n_{\max} = 4$, and $(Q, \tau_c) = (10, 1)$.

For each λ we compute $\rho_S^{\mathrm{exact}}(\lambda)$ from the global Gibbs state by exact diagonalisation and partial trace. We compare it against:

1. the bare Gibbs state $\tau_S \propto e^{-\beta H_S}$;

2. the ultrastrong projected state ρ_{US} from Eq. (7) of Ref. [19] (equivalently the qubit form, Eq. (8) there).

The primary diagnostics are

$$D_\tau = \frac{1}{2}\|\rho_S^{\text{exact}} - \tau_S\|_1, \qquad D_{US} = \frac{1}{2}\|\rho_S^{\text{exact}} - \rho_{US}\|_1, \tag{80}$$

plus the ℓ_1 coherence in the H_S eigenbasis.

The numerical results support the PRL predictions:

1. At $\lambda = 0$, D_τ is numerically zero ($\sim 10^{-16}$), as required.

2. As λ increases, ρ_S^{exact} departs from τ_S and approaches ρ_{US}. For $\beta = 1$, D_{US} drops from 0.1124 at $\lambda = 0$ to 1.99×10^{-3} at $\lambda = 8$, while D_τ increases to 0.1104.

3. Energetic coherence persists in the H_S basis at strong coupling, consistent with Eq. (8) in Ref. [19]: for $\beta = 1$, C_{H_S} increases from 0 at $\lambda = 0$ to 0.218 at $\lambda = 8$.

Figure 1 shows the full coupling scan at $\beta = 1$. Figure 2 shows the temperature dependence ($\beta = 0.5, 1, 2$): in all cases D_{US} is minimised at the largest simulated coupling and remains near 2×10^{-3} at $\lambda = 8$, while the crossover from Gibbs-like to ultrastrong-like behaviour shifts to smaller λ as β increases (approximately $0.6 \to 0.4 \to 0.2$).

A resolution check (low-resolution run: $N_\omega = 2$, $n_{\max} = 3$) changes the $\beta = 1$, $\lambda = 8$ diagnostics only slightly: $|D_{US}^{\text{prod}} - D_{US}^{\text{low}}| = 6.45 \times 10^{-4}$ and $|C_{H_S}^{\text{prod}} - C_{H_S}^{\text{low}}| = 1.25 \times 10^{-3}$, indicating that the qualitative conclusions are robust to the present discretisation.

DISCUSSION

This manuscript is positioned as the direct sequel to Ref. [1]. The earlier paper established the exact commuting Gaussian benchmark; the present one isolates the operator-algebraic obstruction that appears once $[H_Q, f] \neq 0$.

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 to the next stage of the programme: non-Gaussian cumulant extensions and noncommuting finite-bath benchmarks.

The new designability section (Sec. **??**) makes the main constructive consequence explicit for a free-spin core: with a complete pair-resolved channel basis, finite-N all-to-all 2-local coefficient maps are full rank and directly invertible. The numerical component there separates two roles: (i) reconstruction/rank diagnostics for the full all-to-all basis, and (ii) stochastic free-model benchmarking in a dense ZZ sector, where reweighting remains controlled enough to compare against exact thermal ED while also exposing scaling against an MPO/DMRG baseline.

The retained qubit benchmark (Sec.) continues to serve a different purpose: continuity with the weak/ultrastrong asymptotics of Ref. [19]. Together, the two numerical sections split validation into "known asymptotic physics recovery" (qubit) and "constructive many-body designability from free trajectories" (all-to-all construction).

Beyond this, the present formulation makes an informational interpretation of H_{MF} unavoidable. From this perspective, the logarithm acts as a *compression map*. The quenched operator $\bar{\rho}_Q(\beta) = \mathbb{E}_\xi[U_\xi(\beta)]$ is a mixture over history-conditioned propagators, whereas $\tilde{H}_{\text{MF}}(\beta) = -(1/\beta)\log\bar{\rho}_Q(\beta)$ is the unique local object whose Gibbs form reproduces that mixture. The gap between "log of average" and "average of log" is therefore a measure of *how much information about the bath history is lost* when one insists on a single effective Hamiltonian. This is the same structural gap that distinguishes quenched and annealed free energies in disordered statistical mechanics, where one compares $\langle \log Z\rangle$ to $\log\langle Z\rangle$. In the commuting case this gap disappears entirely.

Appendix A: Universal reduction of the moment matrix $C_{nm}(\beta)$

This appendix derives the universal representation (**??**) and gives explicit closed forms for the thermal form factors $S_r(\omega, \beta)$.

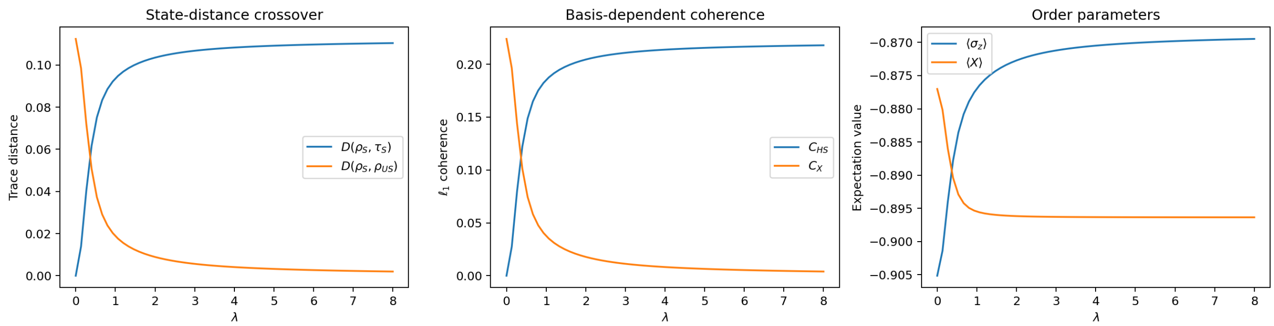

FIG. 1. Single-qubit benchmark at $\beta = 1$: trace-distance crossover, basis-dependent coherence, and expectation-value trends versus coupling strength λ. The exact finite-bath state moves away from the bare Gibbs state and towards the ultrastrong projected state as coupling grows.

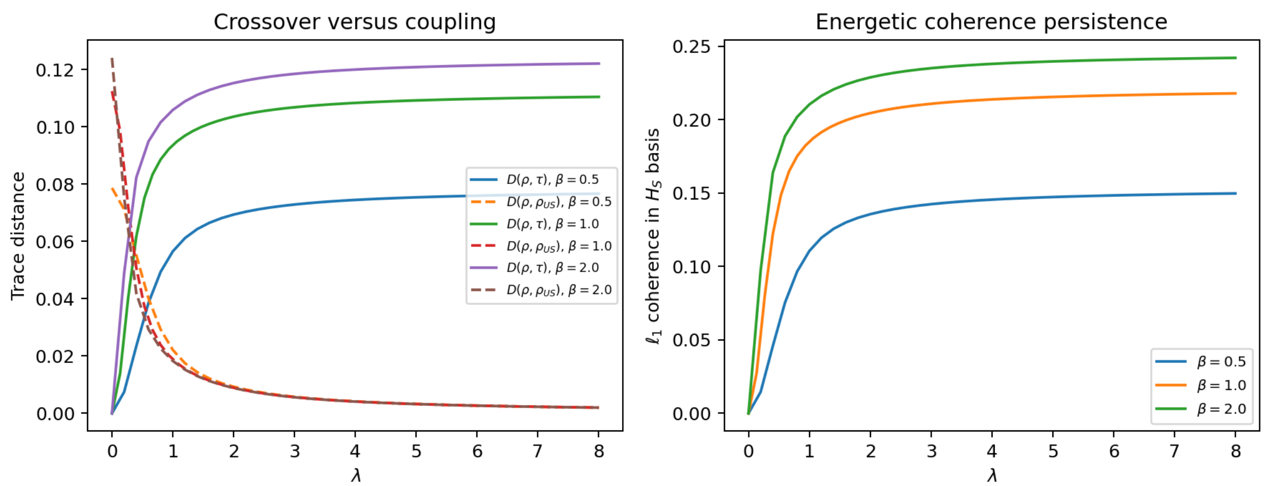

FIG. 2. Temperature comparison ($\beta = 0.5, 1, 2$): left panel shows D_τ (solid) and D_{US} (dashed), right panel shows energetic coherence in the H_S basis. Across temperatures, increasing coupling drives the exact state towards the ultrastrong predicted form while preserving nonzero energetic coherence.

1. Step 1: swap Matsubara sum and spectral integral

Start from

$$C_{nm}(\beta) = \frac{1}{\beta} \sum_{\ell \in \mathbb{Z}} \kappa_\ell \, I_n(\nu_\ell) \, I_m(\nu_\ell)^*, \qquad \nu_\ell = \frac{2\pi\ell}{\beta}, \quad \text{(A1)}$$

and insert the harmonic-bath spectral form (**??**):

$$\kappa_\ell = \frac{2}{\pi} \int_0^\infty d\omega \, \frac{\omega J(\omega)}{\omega^2 + \nu_\ell^2}. \quad \text{(A2)}$$

Assuming the standard UV regularity on $J(\omega)$ that ensures the Gaussian influence functional is well-defined, we may exchange the sum and integral to obtain

$$\begin{aligned} C_{nm}(\beta) &= \frac{2}{\pi} \int_0^\infty d\omega \, \omega J(\omega) \, \Phi_{nm}(\omega, \beta), \\ \Phi_{nm}(\omega, \beta) &\equiv \frac{1}{\beta} \sum_{\ell \in \mathbb{Z}} \frac{I_n(\nu_\ell) I_m(\nu_\ell)^*}{\omega^2 + \nu_\ell^2}. \end{aligned} \quad \text{(A3)}$$

Thus all bath dependence is isolated as the scalar weight $\omega J(\omega)$.

2. Step 2: finite inverse-frequency expansion of $I_n(\nu_\ell)$

For $\ell \neq 0$, bosonic Matsubara frequencies satisfy $e^{i\nu_\ell \beta} = 1$. The integral (**??**) can be evaluated in closed form for $\nu \neq 0$ as

$$I_n(\nu) = \frac{1}{(-i\nu)^{n+1}} \left[1 - e^{i\nu\beta} \sum_{k=0}^{n} \frac{(-i\nu\beta)^k}{k!} \right], \quad \text{(A4)}$$

which for ν_ℓ simplifies to

$$I_n(\nu_\ell) = \frac{1}{(-i\nu_\ell)^{n+1}}\left[1 - \sum_{k=0}^{n}\frac{(-i\nu_\ell\beta)^k}{k!}\right] = -\sum_{p=1}^{n}\frac{\beta^{\,n+1-p}}{(n+1-p)!}\,\frac{1}{(-i\nu_\ell)^p}, \qquad \ell \neq 0. \tag{A5}$$

The $\ell = 0$ value is obtained by continuity,

$$I_n(0) = \frac{\beta^{n+1}}{(n+1)!}. \tag{A6}$$

Define coefficients

$$A_{n,p} \equiv \frac{\beta^{\,n+1-p}}{(n+1-p)!}, \qquad p = 1, \ldots, n, \tag{A7}$$

so that $I_n(\nu_\ell) = -\sum_{p=1}^{n} A_{n,p}(-i\nu_\ell)^{-p}$ for $\ell \neq 0$.

3. Step 3: reduction to even-power Matsubara sums

Split Φ_{nm} into the zero mode and the nonzero modes:

$$\Phi_{nm}(\omega,\beta) = \frac{1}{\beta}\frac{I_n(0)I_m(0)}{\omega^2} + \frac{1}{\beta}\sum_{\ell\neq 0}\frac{I_n(\nu_\ell)I_m(\nu_\ell)^*}{\omega^2+\nu_\ell^2}. \tag{A8}$$

Insert the finite expansion (A5) into the $\ell \neq 0$ term:

$$I_n(\nu_\ell)I_m(\nu_\ell)^* = \sum_{p=1}^{n}\sum_{q=1}^{m} A_{n,p}A_{m,q}\,\frac{1}{(-i\nu_\ell)^p}\,\frac{1}{(+i\nu_\ell)^q}. \tag{A9}$$

Under $\ell \mapsto -\ell$, $\nu_\ell \mapsto -\nu_\ell$ while $\omega^2 + \nu_\ell^2$ is invariant. It follows that contributions with odd $(p+q)$ cancel in the ℓ-sum, leaving only even total powers $p + q = 2r$. Collecting the surviving terms yields the finite reduction

$$\Phi_{nm}(\omega,\beta) = \frac{1}{\beta}\frac{I_n(0)I_m(0)}{\omega^2} + \sum_{r=1}^{\lfloor (n+m)/2\rfloor} \alpha_r^{(nm)}(\beta)\, S_r(\omega,\beta), \tag{A10}$$

where the universal form factors are

$$S_r(\omega,\beta) \equiv \frac{1}{\beta}\sum_{\ell\neq 0}\frac{1}{\nu_\ell^{2r}}\frac{1}{\omega^2+\nu_\ell^2}, \qquad r = 0, 1, 2, \ldots, \tag{A11}$$

and the coefficients are the explicit finite combinatorial contractions

$$\alpha_r^{(nm)}(\beta) \equiv \sum_{\substack{p=1,\ldots,n\\ q=1,\ldots,m\\ p+q=2r}} (-1)^{p+r}\, A_{n,p}A_{m,q}. \tag{A12}$$

Substituting (A10) into (A3) gives the universal representation (**??**).

4. Step 4: closed form for $S_r(\omega,\beta)$

The base sum is standard:

$$S_0(\omega,\beta) = \frac{1}{\beta}\sum_{\ell\neq 0}\frac{1}{\omega^2+\nu_\ell^2} = \frac{1}{2\omega}\coth\!\left(\frac{\beta\omega}{2}\right) - \frac{1}{\beta\omega^2}. \tag{A13}$$

Define also the zeta moments

$$Z_r(\beta) \equiv \frac{1}{\beta}\sum_{\ell\neq 0}\frac{1}{\nu_\ell^{2r}} = \beta^{2r-1}\frac{\zeta(2r)}{(2\pi)^{2r}}, \qquad r \geq 1. \tag{A14}$$

Using the identity

$$\frac{1}{\nu^{2r}(\omega^2+\nu^2)} = \frac{1}{\omega^2}\left(\frac{1}{\nu^{2r}} - \frac{1}{\nu^{2r-2}(\omega^2+\nu^2)}\right), \tag{A15}$$

one obtains the recursion

$$S_r(\omega,\beta) = \frac{1}{\omega^2}\Big(Z_r(\beta) - S_{r-1}(\omega,\beta)\Big), \qquad r \geq 1, \tag{A16}$$

which may be unrolled to the explicit closed form

$$S_r(\omega,\beta) = \sum_{k=0}^{r-1}(-1)^k\frac{Z_{r-k}(\beta)}{\omega^{2(k+1)}} + (-1)^r\frac{S_0(\omega,\beta)}{\omega^{2r}}. \tag{A17}$$

Thus every S_r is an explicit combination of a single thermal function $\coth(\beta\omega/2)$ and a finite set of zeta values $\{\zeta(2), \ldots, \zeta(2r)\}$.

Appendix B: Direct Δ evaluation for the PRL qubit and projector reduction of Eq. (8)

This appendix provides the direct evaluation used in Sec. **??**. We take

$$H_S = \frac{\omega_q}{2}\sigma_z, \qquad X = \cos\theta\,\sigma_z - \sin\theta\,\sigma_x, \tag{B1}$$

and the coupling scaling $J_\lambda(\omega) = \lambda^2 J_0(\omega)$ so that $\kappa_\ell(\lambda) = \lambda^2\kappa_\ell^{(0)}$.

1. Direct-kernel multiplication in Eq. (??)

Using $\tilde{X}(\tau) = e^{\tau H_S} X e^{-\tau H_S}$,

$$\tilde{X}(\tau) = \cos\theta\,\sigma_z - \sin\theta[\cosh(\omega_q\tau)\sigma_x + i\sinh(\omega_q\tau)\sigma_y]\,. \tag{B2}$$

Set $c \equiv \cos\theta$, $s \equiv \sin\theta$, and $u \equiv \tau - \tau'$. Direct Pauli multiplication gives

$$\begin{aligned}\tilde{X}(\tau)\tilde{X}(\tau') = {}& \big[c^2 + s^2\cosh(\omega_q u)\big]\mathbb{I} + s^2\sinh(\omega_q u)\sigma_z \\ &+ cs\big[\sinh(\omega_q\tau) - \sinh(\omega_q\tau')\big]\sigma_x \\ &+ ics\big[\cosh(\omega_q\tau) - \cosh(\omega_q\tau')\big]\sigma_y.\end{aligned} \tag{B3}$$

In Eq. (**??**), however, the bilinear enters as $\mathcal{T}_\tau[\tilde{X}(\tau)\tilde{X}(\tau')]$. Use

$$\mathcal{T}_\tau[AB] = \frac{1}{2}\{A,B\} + \frac{1}{2}\,\mathrm{sgn}(\tau-\tau')[A,B]. \tag{B4}$$

Applying this to the product above gives

$$\begin{aligned}\mathcal{T}_\tau[\tilde{X}(\tau)\tilde{X}(\tau')] = {} & \big[c^2 + s^2\cosh(\omega_q u)\big]\mathbb{I} \\ & + cs\,\mathrm{sgn}(u)\big[\sinh(\omega_q\tau) - \sinh(\omega_q\tau')\big]\sigma_x \\ & + ics\,\mathrm{sgn}(u)\big[\cosh(\omega_q\tau) - \cosh(\omega_q\tau')\big]\sigma_y \\ & + s^2\,\mathrm{sgn}(u)\sinh(\omega_q u)\sigma_z.\end{aligned} \tag{B5}$$

Hence

$$\Delta(\beta,\lambda) = \lambda^2[\alpha_0\mathbb{I} + \delta_x\sigma_x + i\delta_y\sigma_y + \delta_z\sigma_z], \tag{B6}$$

with

$$\alpha_0 = \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K_0(\tau-\tau')\big[c^2 + s^2\cosh(\omega_q(\tau-\tau'))\big], \tag{B7}$$

$$\delta_z = \frac{s^2}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K_0(\tau-\tau')\,\mathrm{sgn}(\tau-\tau')\,\sinh(\omega_q(\tau-\tau')), \tag{B8}$$

$$\delta_x = \frac{cs}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K_0(\tau-\tau')\,\mathrm{sgn}(\tau-\tau')\big[\sinh(\omega_q\tau) - \sinh(\omega_q\tau')\big], \tag{B9}$$

$$\delta_y = \frac{cs}{2}\int_0^\beta d\tau \int_0^\beta d\tau'\,K_0(\tau-\tau')\,\mathrm{sgn}(\tau-\tau')\big[\cosh(\omega_q\tau) - \cosh(\omega_q\tau')\big]. \tag{B10}$$

2. Reduction to one-dimensional direct-kernel moments

Because $K_0(u) = K_0(-u)$, the coefficients reduce exactly to

$$\alpha_0(\beta) = \int_0^\beta du\,(\beta-u)\,K_0(u)\big[c^2 + s^2\cosh(\omega_q u)\big], \tag{B11}$$

$$\delta_z(\beta) = s^2\int_0^\beta du\,(\beta-u)\,K_0(u)\sinh(\omega_q u), \tag{B12}$$

$$\delta_x(\beta) = \frac{cs}{\omega_q}\int_0^\beta du\,K_0(u)\big[\cosh(\beta\omega_q) + 1 - \cosh(\omega_q u) - \cosh\big(\omega_q(\beta-u)\big)\big], \tag{B13}$$

$$\delta_y(\beta) = \frac{cs}{\omega_q}\int_0^\beta du\,K_0(u)\big[\sinh(\beta\omega_q) - \sinh(\omega_q u) - \sinh\big(\omega_q(\beta-u)\big)\big]. \tag{B14}$$

These are exactly Eqs. (**??**)–(**??**) in the main text.

3. Weak-order correction

Let $\tau_S = \frac{1}{2}(\mathbb{I} - \tanh(\beta\omega_q/2)\sigma_z)$ and $\Delta = \lambda^2\Delta_0$. Expanding $\rho \propto e^{-\beta H_S}e^{\Delta}$ to $O(\lambda^2)$ and keeping the Hermitian part gives

$$\delta\rho_{\mathrm{weak}} = \frac{\delta_x}{2}\sigma_x + \frac{1-\tanh^2(\beta\omega_q/2)}{2}\,\delta_z\,\sigma_z, \tag{B15}$$

which is Eq. (**??**). The $i\delta_y\sigma_y$ component contributes to the collapsed finite-coupling product shortcut, but not to this Hermitian weak-order correction.

4. Ordered finite-coupling evaluation used in the benchmark

The finite comparator in Sec. **??** is not the collapsed $e^{-\beta H_S}e^{\Delta}$ product. We evaluate instead

$$\rho_{\mathrm{ord}}(\beta,\lambda) \propto e^{-\beta H_S}\,\mathcal{T}_\tau \exp\left[\lambda^2\int_0^\beta d\tau\int_0^\tau d\tau'\,K_0(\tau-\tau')\,\tilde{X}(\tau)\tilde{X}(\tau')\right], \tag{B16}$$

numerically by deterministic Gaussian quadrature:

1. discretise $\tau \in [0,\beta]$ and build the covariance matrix $C_{ij} = K_0(\tau_i - \tau_j)$;
2. apply a KL decomposition $C \approx VV^\top$ with retained rank r;
3. write the sampled field as $\xi(\tau_i) = \lambda(V\eta)_i$ with independent standard-normal components of η;
4. replace the η-average by tensor Gauss–Hermite quadrature and evaluate each time-ordered trajectory exactly using $\exp[-v\tilde{X}] = \cosh(v)\mathbb{I} - \sinh(v)\tilde{X}$, since $\tilde{X}(\tau)^2 = \mathbb{I}$.

This yields the ordered finite-coupling state used in the figure and CSV outputs.

5. Projector reduction for the PRL ultrastrong qubit state

Take the interaction-axis projectors

$$P_\pm = \frac{1}{2}\left(\mathbb{I} \pm \sigma_{\hat{r}}\right), \qquad \sigma_{\hat{r}} = \cos\theta\,\sigma_z - \sin\theta\,\sigma_x. \tag{B17}$$

Using $H_S = (\omega_q/2)\sigma_z$ and $P_\pm\sigma_z P_\pm = \pm\cos\theta\,P_\pm$,

$$\sum_n P_n H_S P_n = \frac{\omega_q\cos\theta}{2}\left(P_+ - P_-\right) = \frac{\omega_q\cos\theta}{2}\sigma_{\hat{r}}. \tag{B18}$$

Substitution into PRL Eq. (7) gives

$$\rho_{US} = \frac{e^{-(\beta\omega_q\cos\theta/2)\sigma_{\hat{r}}}}{\mathrm{Tr}\big[e^{-(\beta\omega_q\cos\theta/2)\sigma_{\hat{r}}}\big]} = \frac{1}{2}\left[\mathbb{I} - \sigma_{\hat{r}}\tanh\left(\frac{\beta\omega_q\cos\theta}{2}\right)\right], \tag{B19}$$

which is Eq. (??) in the main text.

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