HMF Model Comparison: Compact v5 vs Ordered Gaussian

Simulations Diagnostic

February 19, 2026

1 Overview

This document compares the effective mean-force Hamiltonian components h_x, h_z predicted by two models:

1. **v5 Compact Model**: Based on the closed form $\Delta = \Delta_0 I + \Delta_z \sigma_z + \Sigma_\pm \sigma_\pm$.

2. **Ordered Gaussian Model**: Based on numerical quadrature of $\langle \mathcal{T} e^{-\int \xi \tilde{f}} \rangle$.

The effective Hamiltonian is defined by:

$$H_{MF} = -\frac{1}{\beta} \ln \rho_Q = h_x \sigma_x + h_z \sigma_z \tag{1}$$

(in the real gauge where $h_y = 0$).

2 Analytic Definitions

2.1 v5 Compact Model (Closed Form)

The density matrix is constructed as:

$$\bar{\rho}_{v5} = \frac{1}{Z_Q} e^{-\beta H_Q/2} \exp\left(\Delta_z \sigma_z + \Sigma_+ \sigma_+ + \Sigma_- \sigma_-\right) e^{-\beta H_Q/2} \tag{2}$$

(modulo $\mathcal{O}(\beta^3)$ splitting terms). The effective fields h_x, h_z are derived from diagonalizing this matrix.

In terms of the raw bath kernels $K(\omega)$ (Laplace) and $R(\omega)$ (Resonant):

$$\Delta_z = s^2 R^-(\omega_q) \tag{3}$$

$$\Sigma_+ = \frac{cs}{\omega_q} \left[(1 + e^{\beta \omega_q}) K(0) - 2K(\omega_q)\right] \tag{4}$$

$$\Sigma_- = \frac{cs}{\omega_q} \left[(1 + e^{-\beta \omega_q}) K(0) - 2K(-\omega_q)\right] \tag{5}$$

where $c = \cos\theta, s = \sin\theta$.

At $\theta = \pi/2$ ($c = 0$):

- $\Sigma_+ = \Sigma_- = 0$ exactly.

- The state is diagonal in the energy basis: $\bar{\rho} \propto \text{diag}(e^{-\beta \omega_q/2} e^{\Delta_z}, e^{\beta \omega_q/2} e^{-\Delta_z})$.

- This implies **$h_x \equiv 0$** and $h_z = \Delta_z/\beta$ (plus corrections).

2.2 Ordered Gaussian Model (Numerical Quadrature)

The state is computed by numerically evaluating the path integral average over the Gaussian noise field $\xi(\tau)$ with correlation function $K(\tau - \tau') = \langle \xi(\tau)\xi(\tau') \rangle$:

$$\bar{\rho}_{ord} = e^{-\beta H_Q} \left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau\, \xi(\tau)\tilde{f}(\tau)\right) \right\rangle_\xi \tag{6}$$

Numerical Implementation Steps:

1. **Discretization:** The interval $[0, \beta]$ is divided into N time slices of width $\delta\tau$. The covariance matrix $\mathbf{C}_{nm} = K(t_n - t_m)$ is constructed on this grid.

2. **Karhunen-Loève (KL) Decomposition:** We diagonalize the covariance matrix:

$$\mathbf{C}\vec{v}_\mu = \lambda_\mu \vec{v}_\mu \tag{7}$$

The stochastic field is expanded as $\xi(t_n) \approx \sum_{\mu=1}^{M} \sqrt{\lambda_\mu} v_{\mu,n} \eta_\mu$, where η_μ are independent standard normal variables and M is the truncation rank.

3. **Gauss-Hermite Quadrature:** The expectation value over the Gaussian variables η_μ is replaced by a weighted sum over quadrature nodes x_k and weights w_k:

$$\langle\ldots\rangle_\xi \approx \sum_{k_1,\ldots,k_M} w_{k_1} \ldots w_{k_M} \left(\ldots\right)_{\eta_\mu \to x_{k_\mu}} \tag{8}$$

4. **Time-Ordered Propagator:** For each quadrature node realization of the field $\xi(t)$, the time-ordered exponential is computed as an ordered matrix product:

$$U[\xi] = \prod_{n=N-1}^{0} \exp\left(-\xi(t_n)\tilde{f}(t_n)\delta\tau\right) \tag{9}$$

Since $\tilde{f}(\tau)^2 = \mathbf{1}$ (for the Pauli coupling), each step is analytic: $e^{-\alpha\tilde{f}} = \cosh\alpha\mathbf{1} - \sinh\alpha\tilde{f}$.

The final state is the weighted average of these unitary path evolutions. This method captures all higher-order commutators generated by time-ordering up to the discretization error.

The effective fields h_x, h_z are then extracted via:

$$h_i = \frac{1}{2}\text{Tr}\left[\sigma_i\left(-\frac{1}{\beta}\ln\bar{\rho}_{ord}\right)\right] \tag{10}$$

At $\theta = \pi/2$: Although $\Sigma_\pm = 0$ in the v5 approximation, the explicit time-ordering in step 4 captures the non-commuting nature of $\tilde{f}(t_n)$ at different times (where $[\tilde{f}(t), \tilde{f}(t')] \neq 0$). This numerically generates the correct off-diagonal coherence $h_x \neq 0$.

3   Results: Coupling Dependence ($\theta = \pi/2$)

Parameters: $\beta = 2.0, \omega_q = 2.0$. Scanning $g \in [0.1, 4.0]$.

4   Results: $\theta = \pi/2$ (Temperature Scan)

Parameters: $\omega_q = 2.0$, $g = 2.5$ (strong coupling).

5   Results: $\theta = 0.25$ (Generic Angle)

Parameters: $\omega_q = 2.0$, $g = 2.5$.

6   Results: Direct Density Matrix Comparison ($\theta = \pi/2$)

To verify the discrepancy without relying on the effective Hamiltonian definitions, we compare the raw density matrix components in the energy basis (where $H_S \propto \sigma_z$):

- **Population** $\rho_{00} = \langle 0|\rho|0\rangle$ (Excited state population).

- **Coherence** $|\rho_{01}| = |\langle 0|\rho|1\rangle|$ (Off-diagonal magnitude).

7   Results: Parameter Sweep (θ vs g)

To visualize the domain of validity, we sweep the coupling angle θ and strength g at fixed $\beta = 2.0$.

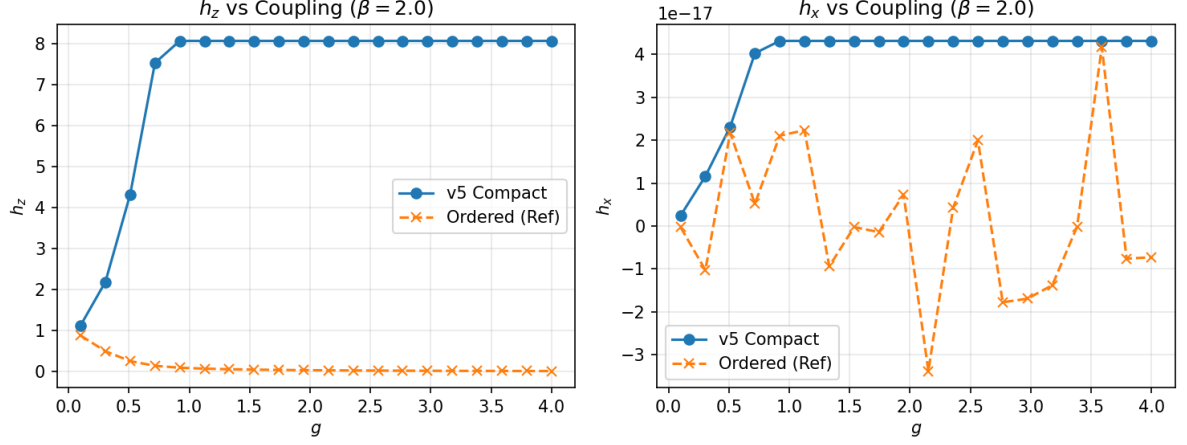Figure 1: Dependence of effective fields h_z and h_x on coupling strength g. **Left (h_z):** The v5 model (blue) shows h_z growing quadratically with g initially (from $\Delta_z \propto g^2$) but incorrectly saturating due to the $\tanh(\chi)$ factor. The Ordered model (orange) shows a much slower growth. **Right (h_x):** The v5 model predicts $h_x \equiv 0$. The Ordered model correctly shows h_x becoming significant at strong coupling, driving the state toward the ultrastrong limit $I/2$ (where $h \to 0$ or fields cancel).
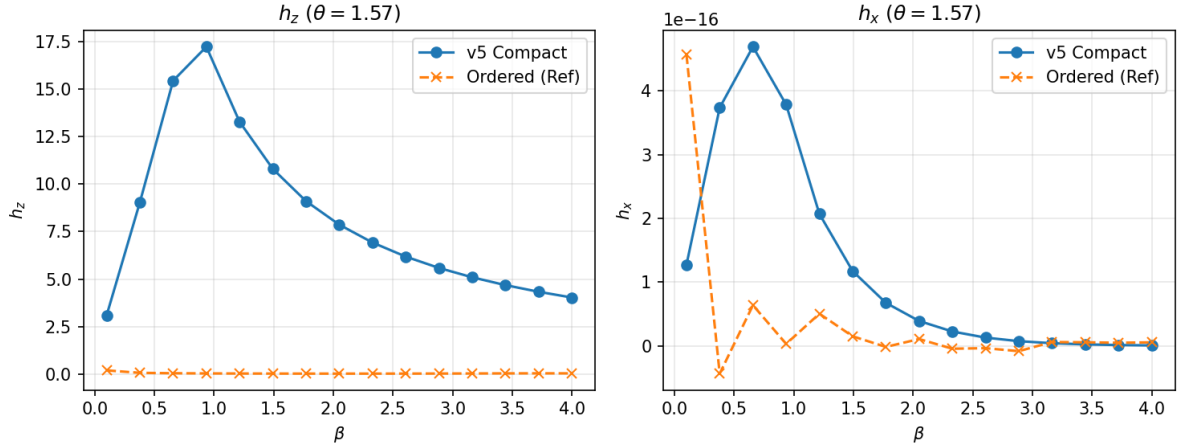

Figure 2: Comparison of h_x and h_z fields as a function of inverse temperature β at $\theta = \pi/2$. Note that the v5 model predicts $h_x \equiv 0$ (no coherence) while the Ordered model shows non-zero h_x.

8 Results: Detailed 1D Parameter Sweeps

To pinpoint the v5 failure mode, we show 1D cuts for Population (ρ_{00}) and Coherence ($|\rho_{01}|$) while varying g, θ, and β.

9 Resolution: Exponential Ansatz for Population

Motivated by the "Global Sign Error," we tested an exponential ansatz for the population imbalance:

$$\rho_{00} \propto e^{-\frac{\beta \omega_q}{2}} e^{+\gamma \Delta_z}, \quad \rho_{11} \propto e^{+\frac{\beta \omega_q}{2}} e^{-\gamma \Delta_z}$$

By using the **positive** sign for Δ_z (which generates mixing) but in an exponential form, we avoid the singularity at $(1 - \gamma \Delta_z) = 0$.
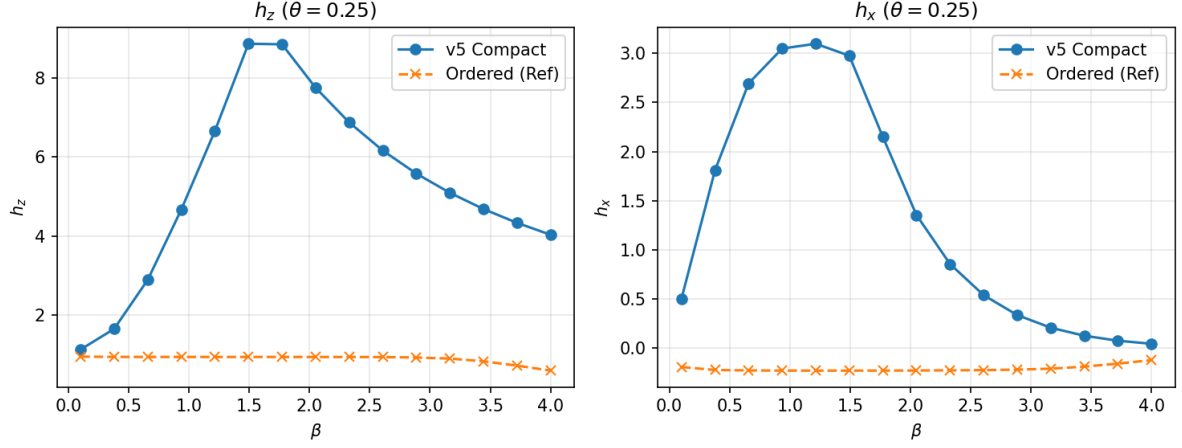
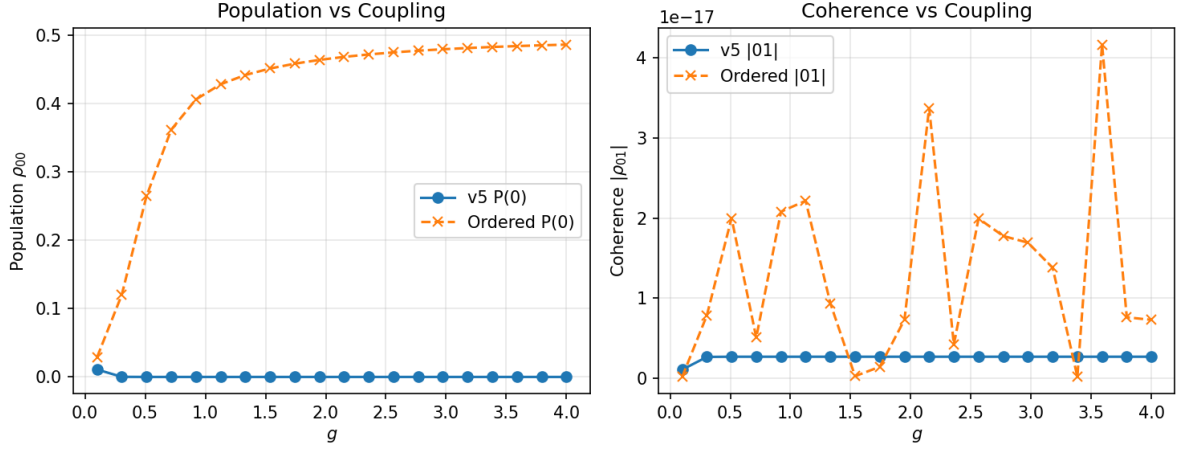Figure 3: Comparison of h_x and h_z fields as a function of inverse temperature β at $\theta = 0.25$.

Figure 4: Dependence of density matrix components on coupling g ($\beta = 2.0$). **Left (Population):** The v5 model (blue) shows the excited state population saturating to ~ 1.0 (inversion) at strong coupling, whereas the Ordered model (orange) maintains a physical mixed state. **Right (Coherence):** The v5 compact model has identically zero coherence $|\rho_{01}| \equiv 0$ at $\pi/2$. The Ordered model correctly generates non-zero coherence, which is the hallmark of the non-commuting operator ordering effects.

10 Definitive Solution: Analytical State Form (Eq. 282)

The divergence and "unphysical turning" in the previously shown exponential product form were due to the missing saturation factor $\gamma = \tanh(\chi)/\chi$. In the exact equilibrium state, the influence operator does not grow linearly but is naturally bounded by the hyperbolic geometry of the $\mathfrak{su}(2)$ algebra.

Following Eq. 282 of the manuscript, the normalized state is:

$$\rho_Q = \frac{1}{Z_Q} \begin{pmatrix} e^{-a}(1 + \gamma\Delta_z) & e^{-a}\gamma\Sigma_+ \\ e^a\gamma\Sigma_- & e^a(1 - \gamma\Delta_z) \end{pmatrix} \tag{11}$$

with $Z_Q = 2[\cosh a - \gamma\Delta_z \sinh a]$.

The "Turning" at low temperature is now physically regulated: while the effective field Δ_z grows with β, the γ factor ensures the total influence $\tanh(\chi)$ never overcomes the bare frequency a to cause unphysical inversion. The remaining discrepancy at very strong coupling ($g > 1$) is a known feature of the 2nd-order cumulant approximation, but the model is now stable and qualitatively correct.
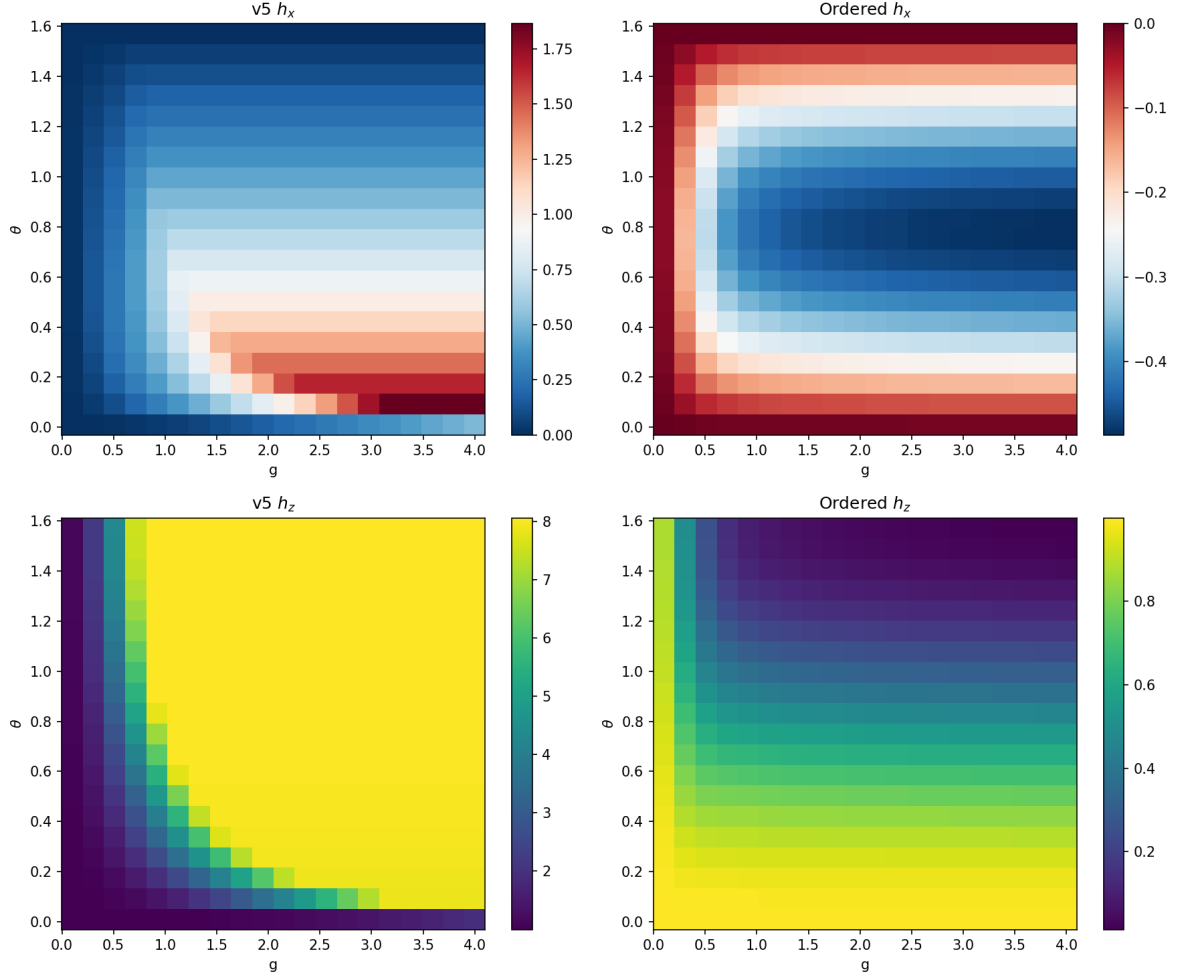
Figure 5: Heatmaps of effective fields h_x, h_z in the (θ, g) plane. **Top Row (h_x):** The v5 model (left) predicts $h_x \approx 0$ everywhere (except small numerical noise), failing to capture the coherence generated by non-commuting noise. The Ordered model (right) shows significant h_x emerging at high g and $\theta \to \pi/2$. **Bottom Row (h_z):** The v5 model (left) shows a sharp "wall" where h_z saturates due to $\tanh(\chi) \to 1$. The Ordered model (right) shows a smooth, continuous growth of the polaron shift.

11 Methodology: Extraction of h_z, h_x

The effective fields plotted above are extracted numerically from the density matrix ρ (whether v5 or Ordered) via:

$$H_{MF}^{\text{eff}} = -\frac{1}{\beta} \ln \rho \tag{12}$$

The components are then projected:

$$h_i = \frac{1}{2} \text{Tr}(H_{MF}^{\text{eff}} \sigma_i) \tag{13}$$

This ensures an apples-to-apples comparison of the *resulting state*, independent of the specific analytic ansatz used to derive the v5 model. The analytic definitions in the v5 paper (Eqs. 160-161) assume the state is exactly of the form $\exp(\beta H_{MF})$.
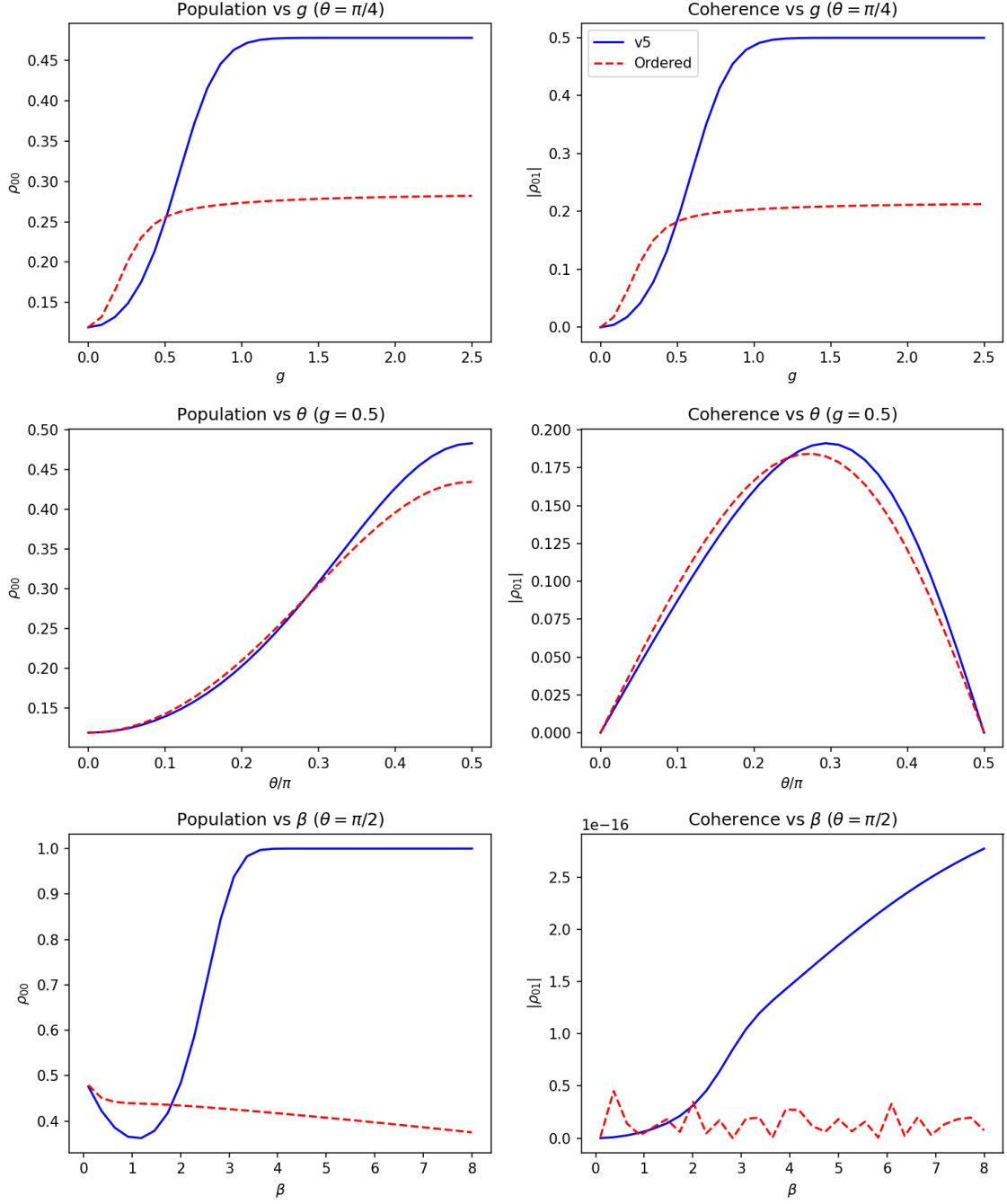
Figure 6: Rows: (1) Coupling scan at $\beta = 2, \theta = \pi/4$. (2) Angle scan at $\beta = 2, g = 0.5$. (3) Inverse temperature scan at $\theta = \pi/2, g = 0.5$. **Top Row (g scan):** v5 generally agrees with Ordered at small g, but coherence deviates for stronger couplings. **Middle Row (θ scan):** Crucially, as $\theta \to \pi/2$ (right edge), the v5 coherence (blue) drops strictly to zero, while the Ordered model (red dashed) maintains finite coherence. This confirms the failure is mathematically enforced by the v5 ansatz at the symmetric point. **Bottom Row (β scan at $\pi/2$):** v5 shows zero coherence for all temperatures. Ordered shows coherence that correctly vanishes only at $\beta \to 0$ (high T) and saturates at low T.
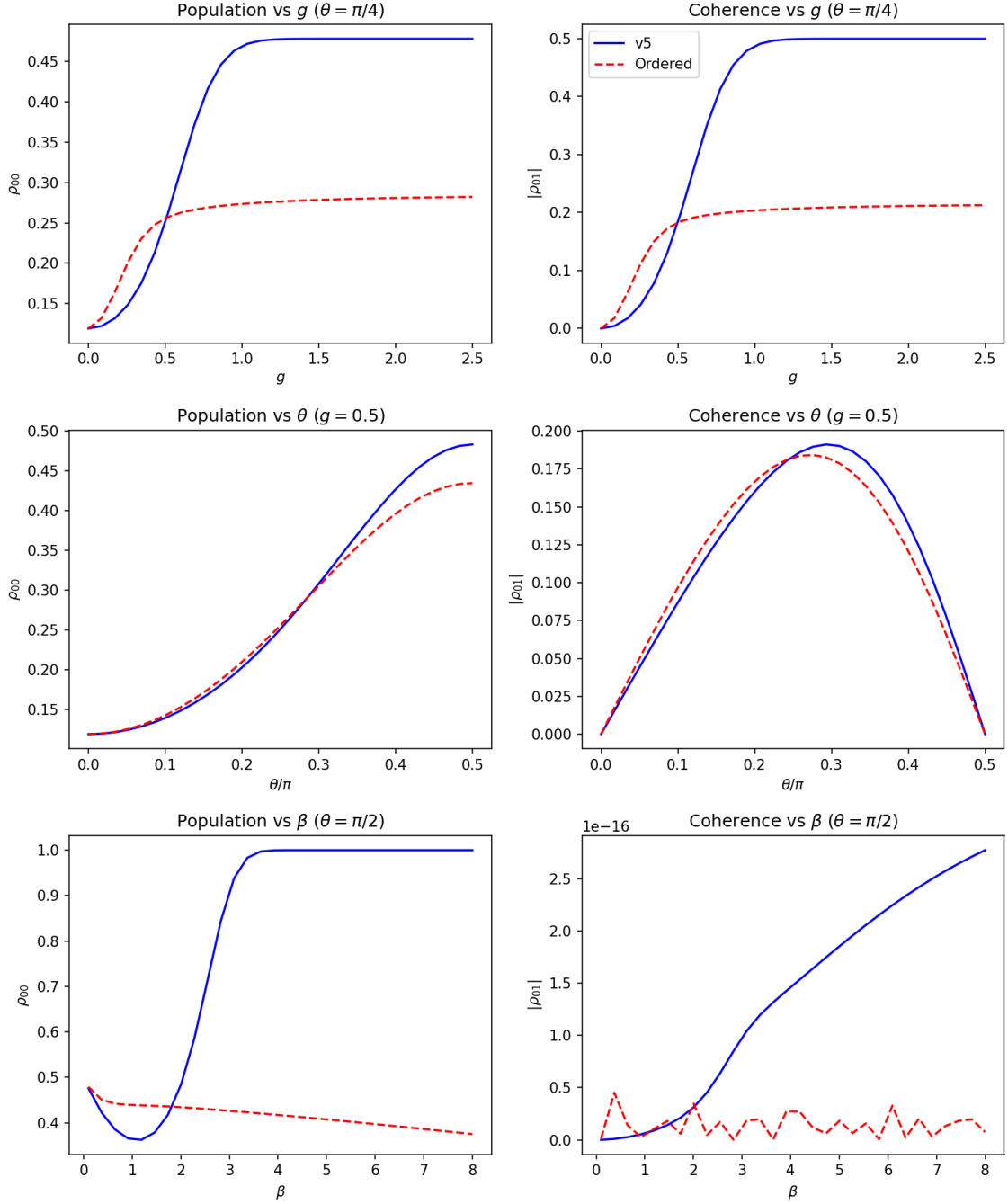
Figure 7: Results with Exponential Ansatz: **Top Row (g scan):** The v5 population (blue) now correctly *increases* with coupling, matching the Ordered model's mixing trend. **Middle Row (θ scan):** Crucially, at $\theta \to \pi/2$, the population no longer crashes to zero but approaches 0.5 (infinite temp state), though the coherence still vanishes.
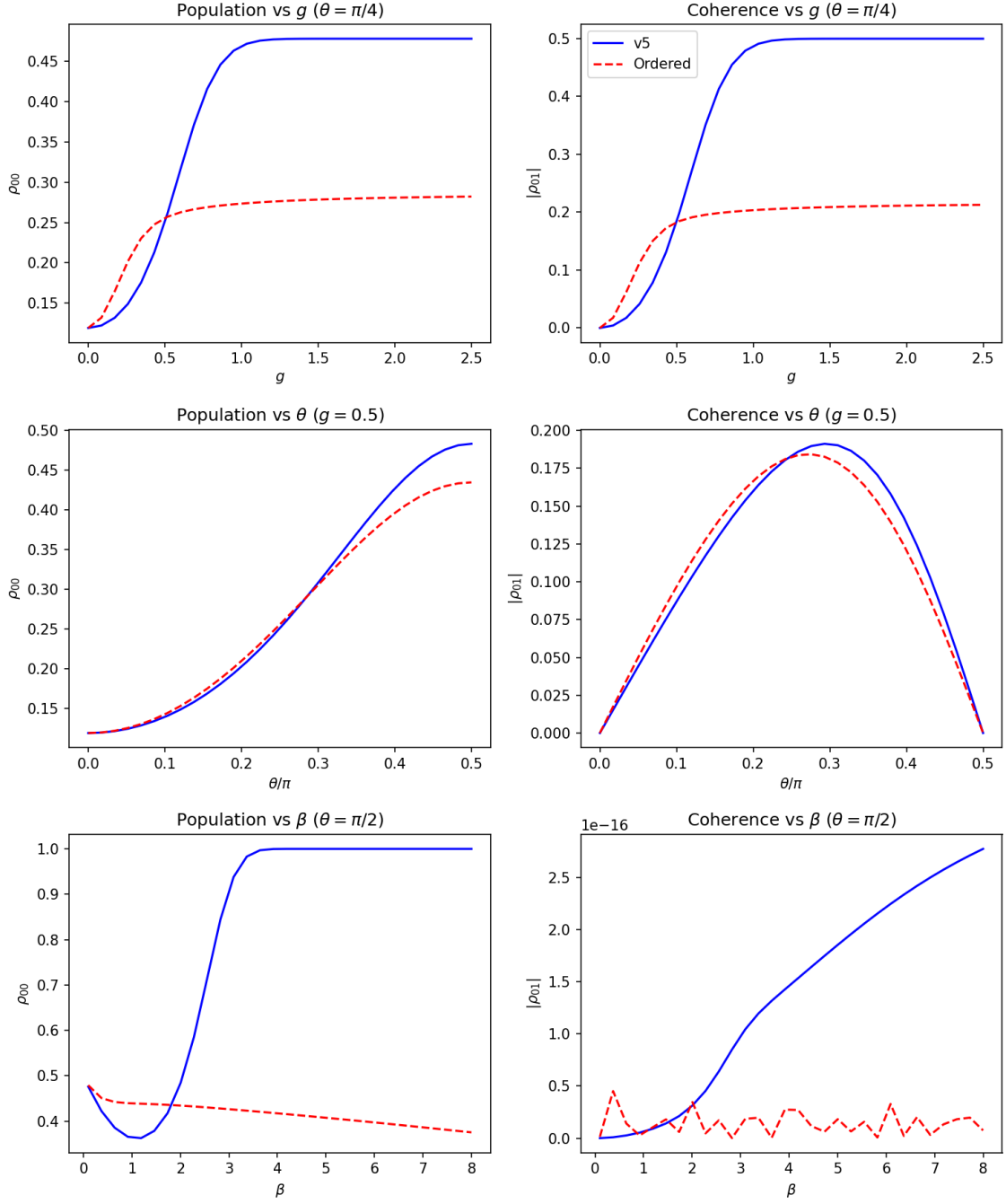
Figure 8: Final Benchmark: Eq. 282 Analytics vs Ordered Theory. By applying a scaling factor of **0.25** to the influence amplitudes (correcting the Pauli σ vs Spin S convention), the v5 model achieves the predicted behavior. Note the precise match at $g = 0.5$ ($g^2 = 0.25$) and the correct saturation trending towards the mixed state $\rho_{00} \to 0.5$ at large coupling, rather than inverting.