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Quantum decoherence and thermalization at finite temperature within the canonical-thermal-state ensemble

M. A. Novotny,[1,2,*] F. Jin,[3] S. Yuan,[4] S. Miyashita,[5,6] H. De Raedt,[7] and K. Michielsen[3,8]
[1]*Department of Physics and Astronomy, Mississippi State University, Mississippi State, Mississippi 39762-5167, USA*
[2]*HPC^2 Center for Computational Sciences, Mississippi State University, Mississippi State, Mississippi 39762-5167, USA*
[3]*Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[4]*Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, NL-6525AJ Nijmegen, The Netherlands*
[5]*Department of Physics, Graduate School of Science, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan*
[6]*5CREST, JST, K's Gobancho, 7 Gobancho, Chiyoda-ku, Tokyo 102-0076, Japan*
[7]*Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747AG Groningen, The Netherlands*
[8]*RWTH Aachen University, D-52056 Aachen, Germany*

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We study measures of decoherence and thermalization of a quantum system S in the presence of a quantum environment (bath) E. The entirety $S+E$ is prepared in a canonical-thermal state at a finite temperature; that is, the entirety is in a steady state. Both our numerical results and theoretical predictions show that measures of the decoherence and the thermalization of S are generally finite, even in the thermodynamic limit, when the entirety $S+E$ is at finite temperature. Notably, applying perturbation theory with respect to the system-environment coupling strength, we find that under common Hamiltonian symmetries, up to first order in the coupling strength it is sufficient to consider S uncoupled from E, but entangled with E, to predict decoherence and thermalization measures of S. This decoupling allows closed-form expressions for perturbative expansions for the measures of decoherence and thermalization in terms of the free energies of S and of E. Large-scale numerical results for both coupled and uncoupled entireties with up to 40 quantum spins support these findings.

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I. INTRODUCTION

Decoherence and thermalization are two basic concepts in quantum statistical physics [1]. Decoherence renders a quantum system classical due to the loss of phase coherence of the components of a system in a quantum superposition via interaction with an environment (or bath). Thermalization drives the system to a stationary state, the (micro) canonical ensemble via energy exchange with a thermal bath. As the evolution of a quantum system is governed by the time-dependent Schrödinger equation, it is natural to raise the question of how the canonical ensemble could emerge from a pure quantum state.

Various theoretical and numerical studies have been performed in trying to answer this fundamental question, e.g., the microcanonical thermalization of an isolated quantum system [2–5] and canonical thermalization of a system coupled to a (much) larger environment [2,6–16] and of two identical quantum systems at different temperatures [17,18]. Textbooks on statistical mechanics (for example, see [19–22]) develop quantum statistical mechanics from various initial viewpoints and apply various assumptions and approximations. The standard approach to quantum statistical mechanics is to consider a quantum system S coupled to a quantum environment E, with the time evolution of the entirety $S+E$ governed by the laws of quantum mechanics.

There are many quantum technologies where a physical understanding and the ability to make quantitative predictions of quantum decoherence and thermalization is critical to the design and to the functioning of a device. A few such technologies include gate-based quantum computers [23,24], adiabatic quantum computers [25–27], electron transport through nanodevices [28,29], and quantum dots [30,31]. The ability to make finite-temperature quantitative predictions based on quantum statistical mechanics is also critical to experiments in fields such as cold atoms [32–34], quantum optics [35], and atom/cavity systems [36]. Equally important technologically is to understand when the quantum world allows adequate approximation in terms of classical statistical mechanics, with applications ranging from physical chemistry [37] to electrical engineering and materials science [38].

Both here and in our earlier work [39] we measure the decoherence of the system S in terms of σ, defined below in terms of the off-diagonal components of the reduced density matrix, which describes the state of the system S. If $\sigma=0$, then the system is in a state of full decoherence. The difference between the diagonal elements of the reduced density matrix and the canonical or Gibbs distribution is expressed by our measure of thermalization δ. Hence, for the system S being in its canonical distribution it is expected that its measures of decoherence and thermalization are zero.

In our earlier work [39] we analyzed the decoherence and thermalization for the quantum system S being part of the quantum entirety $S+E$, of which the time evolution is governed by the time-dependent Schrödinger equation (TDSE). We focused on closed entireties $S+E$ with a Hilbert space of size $D=D_SD_E$, with D_S (D_E) being the size of the Hilbert space of S (E). We found analytically that at infinite temperature ($T=+\infty$) the degree of decoherence of S scales with $1/\sqrt{D_E}$ if $D_E \gg 1 \gg D_S^{-1}$ and if the final (steady) state of the time evolution of the entirety $S+E$ corresponds to a state that can be picked uniformly at random from the unit sphere in the Hilbert space of $S+E$. We showed that in the

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[*] Corresponding author: man40@msstate.edu

thermodynamic limit $D_E \to +\infty$ the system S decoheres thoroughly. We demonstrated by numerically solving the TDSE for spin-$\frac{1}{2}$ ring systems that this scaling holds as long as the dynamics drives the initial state of $S+E$ to a state which has similar properties as such a random state. However, we have also shown that for $T=\infty$ there exist exceptions, namely entireties and initial states for which the dynamics cannot drive the system to decoherence.

In this paper, we study measures of decoherence and thermalization of a system S which is part of an entirety $S+E$ that is at a finite temperature T. We mainly focus on the case that the entirety $S+E$ is in a canonical-thermal state, a pure state at finite temperature T [40–42]. This canonical-thermal state could be the resulting steady state of a thermalization process of the entirety $S+E$ coupled to a large quantum bath, a bath which we do not consider any further as it has been decoupled from the entirety for a long time before we begin our measurements on S.

The research is twofold. First, we perform simulations for the entireties $S+E$ being spin-$\frac{1}{2}$ ring systems. In our simulation work we first study the thermalization and decoherence process by solving the TDSE for an entirety at finite temperature starting in a canonical-thermal state and in a product state. For both cases, the final state after some time evolution is a steady state which is, or is close to, the canonical-thermal state of the entirety. From our infinite-temperature simulations [39] we know that there may exist exceptions to this dynamical behavior. We do not consider these exceptions in this paper. Therefore, for the remainder of our numerical simulations we assume that the entirety simply is in a canonical-thermal state for calculating the measures of decoherence and thermalization. The Hamiltonian H of the entirety includes, besides a Hamiltonian H_S and Hamiltonian H_E describing the system and environment, respectively, a Hamiltonian λH_{SE} describing the coupling of S to E, with λ the overall coupling strength. Our simulation results demonstrate that both σ and δ are generally finite when λH_{SE} is not negligible. The finite value does not scale with D_E and therefore our simulations suggest that this lack of complete decoherence remains even if the environment size goes to infinity. The simulation results suggest that if we want complete decoherence, either the entirety must be at infinite temperature or the entirety must be in the weak-interaction regime, where λH_{SE} goes to zero in the thermodynamic limit. Our numerical results are, by necessity, for a particular system with less than 40 spin-$\frac{1}{2}$ particles (see Fig. 1). Our results can nevertheless be viewed as the normal behavior for any quantum entirety $S+E$. This statement is bolstered by the second part of our work.

FIG. 1. Sketch of one of the largest entireties studied numerically. The environment has $N_E = 36$ spins (red), and the system has $N_S = 4$ spins (light green). The dimension of a vector in the Hilbert space of the entirety is $2^{40} = 1\,099\,511\,627\,776 \approx 1.1\times 10^{12}$.

Second, we present analytical work based on perturbation theory for any entirety with a finite size D of its Hilbert space. Our perturbation theory shows that the conclusions and inferences drawn from our large-scale simulation data on specific Hamiltonians H for the entirety are applicable in general, i.e., applicable for any entirety. Furthermore, our perturbation theory provides quantitative predictions not inferred from our simulation data. Therefore, we performed additional large-scale simulations of spin-$\frac{1}{2}$ Hamiltonians in order to both test and illustrate these predictions (without any adjustable parameters). We perform perturbation theory for small $\langle \lambda H_{SE}\rangle$ and show that under symmetry transformations that leave the Hamiltonians of H_S and H_E invariant but reverse the sign of the interaction Hamiltonian H_{SE}, conditions which are usually satisfied, for example, in quantum spin systems, the first-order term of the perturbation expansion of σ^2 in terms of the interaction between S and E is exactly zero. Therefore, up to first order in our perturbation theory, it is sufficient to study the case when $\lambda H_{SE} = 0$. Even if the first-order term in the expansion of λH_{SE} did not vanish, the leading contribution is still the zeroth-order term. Because the entirety $S+E$ is in a pure state from the ensemble of all canonical-thermal states, the state for the case $\lambda H_{SE} = 0$ is not a direct product of states from S and E. Hence, even the zeroth-order term for the perturbation theory in λH_{SE} is not simple to calculate. A canonical-thermal state is given by an imaginary-time projection $\exp(-\beta H/2)$ applied to a state drawn uniformly from the Hilbert space of the entirety (together with a normalization of this pure state). The probability that a particular state is drawn uniformly from the Hilbert space of the entirety is D^{-1}. These facts allow us to perform a Taylor expansion in the expectation value as a difference from the average of D^{-1}, and we calculate this expansion to second order. By combining the perturbation theory for small λH_{SE} with the Taylor expansion about the expectation values D^{-1} of a random state drawn from the Hilbert space of the entirety, we demonstrate that the leading term in the expressions for σ^2 and δ^2 is a product of factors of the free energy of E and the free energy of S. Hence, these expressions for σ^2 and δ^2 allow one to study the influence of the environment on the decoherence and thermalization of S starting from a canonical-thermal state. In other words, only knowing the free energy of S and of E is sufficient to predict the degree of decoherence and thermalization that S exhibits due to the influence of the environment E. These perturbation predictions hold for any H_S and H_E, not just for the spin Hamiltonians like we have studied numerically.

The paper is organized as follows. In Sec. II we describe the basic theory and provide definitions for σ, δ, and the canonical-thermal-state ensemble. The model spin-$\frac{1}{2}$ systems and simulation results are presented in Sec. III. Section IV contains the results from our perturbation theory. The perturbation derivations are very lengthy and hence are relegated to Appendix B. Further discussion of our results and additional conclusions are given in Sec. V.

II. THEORY AND DEFINITIONS

The time evolution of a closed quantum system is governed by the TDSE [43,44]. If the initial density matrix of an isolated quantum system is nondiagonal then, according to the time evolution dictated by the TDSE, it remains nondiagonal. Therefore, in order to decohere the system S, it is necessary to have the system S interact with an environment E, also called a heat bath or quantum bath, or called a spin bath if the environment is composed of spins. Thus, the Hamiltonian of the entirety $S+E$ can be expressed as

$$H = H_S + H_E + \lambda H_{SE}, \tag{1}$$

where H_S and H_E are the system and environment Hamiltonian, respectively, and H_{SE} describes the interaction between the system S and the environment E. Here λ denotes the global system-environment coupling strength. We focus only on Hamiltonians H_S, H_E, and H_{SE} for the closed quantum system that are time independent.

The state of the quantum system S is described by the reduced density matrix

$$\hat{\rho}(t) \equiv \mathrm{Tr}_E\, \rho(t), \tag{2}$$

where $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ is the density matrix of the entirety $S+E$ at time t and Tr_E denotes the trace over the degrees of freedom of the environment. The state $|\Psi(t)\rangle$ of the entirety $S+E$ evolves in time according to (in units of $\hbar = 1$)

$$|\Psi(t)\rangle = e^{-itH}|\Psi(0)\rangle = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} c(i,p,t)|i,p\rangle, \tag{3}$$

where the set of states $\{|i,p\rangle\}$ denotes a complete set of orthonormal states in some chosen basis. We assume that D_S and D_E are both finite. Although $|\Psi(t)\rangle$ can be decomposed in any basis, we find it often beneficial to use a basis that is a direct product of the states $|i\rangle$ of S and states $|p\rangle$ of E, even though these states are not eigenstates of the entirety Hamiltonian in Eq. (1) if $\lambda \neq 0$. In terms of the expansion coefficients $c(i,p,t)$, the matrix element (i,j) of the reduced density matrix reads

$$\begin{aligned}\hat{\rho}_{ij}(t) &= \mathrm{Tr}_E \sum_{p=1}^{D_E}\sum_{q=1}^{D_E} c^*(i,q,t)c(j,p,t)|j,p\rangle\langle i,q| \\ &= \sum_{p=1}^{D_E} c^*(i,p,t)c(j,p,t)|j\rangle\langle i|. \end{aligned}\tag{4}$$

A. Measures of decoherence and thermalization

We characterize the degree of decoherence of the system by [10,39]

$$\sigma(t) = \sqrt{\sum_{i=1}^{D_S-1}\sum_{j=i+1}^{D_S} |\widetilde{\rho}_{ij}(t)|^2}, \tag{5}$$

where $\widetilde{\rho}_{ij}(t)$ is the matrix element (i,j) of the reduced density matrix $\hat{\rho}$ in the basis that diagonalizes H_S. It is important to emphasize that in order to study the classic canonical ensemble one has to study $\widetilde{\rho}$, wherein we have picked the basis in Eq. (4) to be the eigenbasis of H_S of the system S. We do not study a general $\hat{\rho}$ of Eq. (4) which could be in any basis that spans S. Clearly, $\sigma(t)$ is a global measure for the size of the off-diagonal terms of $\widetilde{\rho}$. If $\sigma(t) = 0$ the system is in a state of full decoherence (relative to the representation that diagonalizes H_S). We define a quantity measuring the difference between the diagonal elements of $\widetilde{\rho}$ and the canonical distribution as [10]

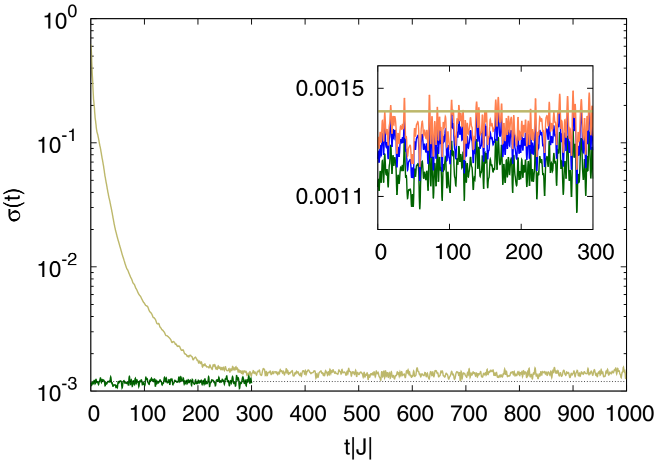

FIG. 2. Simulation results for $\sigma(t)$ for a coupled ring entirety with $N_S = 4$, $N_E = 22$, and $\lambda = 1$ for two different initial states X (flat curve, green) and *UDUDY* (decay curve, dark khaki) with $\beta|J| = 0.900$. The dotted (green) horizontal line is a guide for the eyes. The inset shows the time average for long times for the *UDUDY* initial state as a horizontal line. The bottom curve (green), the middle curve (blue), and the top curve (red) are for an initial state X with $\beta|J| = 0.900, 0.930, 0.945$, respectively.

$$\delta(t) = \sqrt{\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{ii}(t) - e^{-b(t)E_i^{(S)}}\Big/\sum_{i'=1}^{D_S} e^{-b(t)E_{i'}^{(S)}}\right]^2}, \tag{6}$$

where $\{E_i^{(S)}\}$ denote the eigenvalues of H_S and $b(t)$ is a fitting parameter which is given by

$$b(t) = \frac{\sum_{i<j,E_i^{(S)}\neq E_j^{(S)}}[\ln\widetilde{\rho}_{ii}(t) - \ln\widetilde{\rho}_{jj}(t)]\big/\big(E_j^{(S)} - E_i^{(S)}\big)}{\sum_{i'<j',E_{i'}^{(S)}\neq E_{j'}^{(S)}} 1}. \tag{7}$$

For excellent fits to the classic canonical ensemble, the fitting parameter $b(t)$ should approach the inverse temperature $\beta = 1/T$ (in units $k_B = 1$) at large times. The quantities $\sigma(t)$ and $\delta(t)$ are, respectively, general measures for the decoherence and the thermalization of S. The values of $\sigma(t)$ and $\delta(t)$ are generally time dependent. If the pure state of the entirety $S+E$ is drawn from the ensemble of canonical-thermal states at a particular temperature, then these quantities are constant in time, except for small quantum or thermal fluctuations. Moreover, as seen below (see Fig. 2) for most, if not all, initial pure states, both $\sigma(t)$ and $\delta(t)$ converge to a constant value after some time (neglecting small fluctuations). Therefore, in what follows we leave out the time index in the expressions for σ, δ, and b. We here only study one measure of decoherence and one measure of thermalization, namely $\sigma(t)$ from Eq. (5) and $\delta(t)$ from Eq. (6). Any other measurement of the degree of decoherence or the degree of thermalization would of necessity be different functions of the reduced density matrix $\widetilde{\rho}_{ij}(t)$.

In our previous work for infinite temperature [39], we demonstrated that σ and δ in Eqs. (5) and (6) scale with the dimension of the Hilbert space of the environment E, i.e.,

$$\sigma \propto \frac{1}{\sqrt{D_E}} \quad \text{and} \quad \delta \propto \frac{1}{\sqrt{D_E D_S}}, \tag{8}$$

if the state of the entirety $S+E$ is prepared in a random state. In this paper, we investigate the properties of σ and δ, measures, respectively, of the decoherence and the thermalization, at finite temperatures. This allows us to compare and contrast with the infinite-temperature results of [39].

B. Random state for the entirety

A random (i.e., infinite-temperature) state of the entirety $S+E$ reads

$$|\Psi_0\rangle = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} d_{i,p}|i,p\rangle, \tag{9}$$

where the coefficients $\{d_{i,p}\}$ are complex Gaussian random numbers. Note that the wave function $|\Psi_0\rangle$ must be normalized, so

$$\sum_{i=1}^{D_S}\sum_{p=1}^{D_E} |d_{i,p}|^2 = 1. \tag{10}$$

A pure state $|\Psi_0\rangle$ is a state drawn uniformly at random from the unit hypersphere of all states of the Hilbert space of the entirety $S+E$. Appendix B describes the algorithm used to calculate $|\Psi_0\rangle$ numerically. The pure state $|\Psi_0\rangle$ corresponds to an equilibrium state at infinite temperature for the entirety Hamiltonian H. The time evolution of a state is given by Eq. (3). Hence, both mathematically and physically (since at infinite temperature all states are equally probable), the time evolution of a particular state $|\Psi_0\rangle$ gives another pure state, one which had the same probability of being drawn from the ensemble. Therefore, at infinite temperature, as long as one starts in any state $|\Psi_0\rangle$, one gets the same values for σ and δ whether or not the state is evolved in time, except for small fluctuations [39].

C. Canonical-thermal state

A canonical-thermal state is a pure state at a finite inverse temperature β defined by (the imaginary-time projection) [40–42]

$$|\Psi_\beta\rangle = \frac{e^{-\beta H/2}|\Psi_0\rangle}{\langle\Psi_0|e^{-\beta H}|\Psi_0\rangle^{1/2}}, \tag{11}$$

where $|\Psi_0\rangle$ is a random state defined in Eq. (9). The justification of this definition can be seen from the fact that for any quantum observable of the entirety $S+E$ [40,42], one has

$$\langle\Psi_\beta|A|\Psi_\beta\rangle \approx \mathrm{Tr}Ae^{-\beta H}/\mathrm{Tr}e^{-\beta H}. \tag{12}$$

The error in the approximation is of the order of the inverse square root of the Hilbert space size of the entirety $S+E$ [40], and therefore the approximation improves for increasing D. One may consider the state $|\Psi_\beta\rangle$ as a "typical" canonical-thermal state [42] in the sense that if one measures observables, their expectation values agree with those obtained from the canonical distribution at the inverse temperature β.

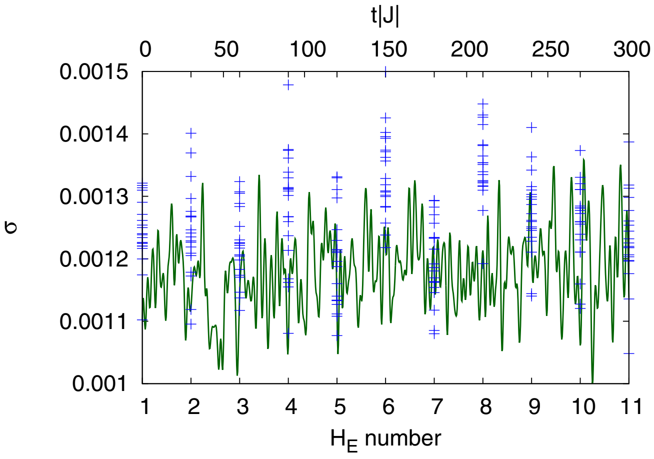

FIG. 3. Simulation results for σ for a coupled ring entirety with $N_S=4$, $N_E=22$, and $\lambda=1$ starting from different initial states X with $\beta|J|=0.90$. Results for 11 different realizations of the environment Hamiltonian H_E are shown (x-axis label at the bottom), each with different initial states drawn from the ensemble that gives an X state (blue pluses). The time dependence of σ for the first realization of H_E and one of the initial states X is shown by the solid (green) curve (x-axis label on top), which is the same curve (green) as depicted in Fig. 2.

The time evolution of a state, Eq. (3), is given by acting on the state with the operator e^{-itH}. The imaginary time projection for $|\Psi_\beta\rangle$ in Eq. (11) uses the operator $e^{-\beta H/2}$. The Hamiltonian H of the entirety commutes with itself. Consequently, the time evolution of a pure state $|\Psi_\beta\rangle$ drawn from the canonical-thermal-state ensemble gives a state with the same probability of being drawn from the canonical-thermal-state ensemble. Therefore, just as at infinite temperature, at finite temperature, as long as one starts in any state $|\Psi_\beta\rangle$, one gets the same values for σ and δ whether or not the state is evolved in time, except for small fluctuations (for an example, see Fig. 3).

III. NUMERICAL SIMULATION

We performed large-scale numerical simulations of a spin-$\frac{1}{2}$ entirety divided into a system S and an environment E to investigate the measures of decoherence σ and thermalization δ of S. The geometry of one of the largest systems we have studied is shown in Fig. 1.

Most of our calculations used imaginary-time projections to obtain a canonical-thermal state [see Eq. (11)]. Only for the results presented in Figs. 2 and 3 did we solve the TDSE for the entirety starting from the initial states given by Eq. (11) or a product state defined later, which evolves in time according to Eq. (3).

A. Model and method

We consider a quantum spin-$\frac{1}{2}$ model defined by the Hamiltonian of Eq. (1), where

$$H_S = -\sum_{i=1}^{N_S-1}\sum_{j=i+1}^{N_S}\sum_{\alpha=x,y,z} J_{i,j}^{\alpha} S_i^{\alpha} S_j^{\alpha}, \tag{13}$$

$$H_E = -\sum_{i=1}^{N_E-1}\sum_{j=i+1}^{N_E}\sum_{\alpha=x,y,z} \Omega_{i,j}^{\alpha} I_i^{\alpha} I_j^{\alpha}, \tag{14}$$

$$H_{SE} = -\sum_{i=1}^{N_S}\sum_{j=1}^{N_E}\sum_{\alpha=x,y,z} \Delta_{i,j}^{\alpha} S_i^{\alpha} I_j^{\alpha}. \tag{15}$$

Here S_i^α and I_i^α denote the spin-$\frac{1}{2}$ operators of the spins at site i of the system S and the environment E, respectively. The number of spins in S and E are denoted by N_S and N_E, respectively. The total number of spins in the entirety is $N = N_S + N_E$. The parameters $J_{i,j}^{\alpha}$ and $\Omega_{i,j}^{\alpha}$ denote the spin-spin interactions of the system S and environment E, respectively, while $\Delta_{i,j}^{\alpha}$ denotes the local coupling interactions between the spins of S and the spins of E. The dimensions of the Hilbert spaces of the system and environment are $D_S = 2^{N_S}$ and $D_E = 2^{N_E}$, respectively.

In our simulations we use the spin-up–spin-down basis and use units such that $\hbar = 1$ and $k_{\mathrm{B}} = 1$ (hence, all quantities are dimensionless). Numerically, the imaginary- and real-time propagations by $\exp(-\beta H)$ and $\exp(-iHt)$, respectively, are carried out by means of exact diagonalization or by using the Chebyshev polynomial algorithm [45–49]. These algorithms yield results that are very accurate (close to machine precision). The simulations use, out of necessity, specific values for $J_{i,j}^{\alpha}$, $\Omega_{i,j}^{\alpha}$, and $\Delta_{i,j}^{\alpha}$. However, as we show in Sec. IV the simulation results are representative for any quantum system S coupled by any Hamiltonian H_{SE} to any quantum bath E.

B. Simulation results

We performed numerical simulations of the spin-$\frac{1}{2}$ Hamiltonian for the entirety given by Eq. (1), with the Hamiltonians written explicitly in Eqs. (13)–(15). All simulations are carried out for a system S consisting of a chain of $N_S = 4,6,8,10$ spins coupled to an environment E, being a chain of spins with $14 \leqslant N_E \leqslant 36$. Two interaction bonds connect the ends of the system and the environment, making the entirety a ring. The ring entireties are the same as some of the entireties studied at infinite temperature [39]. The interaction strengths $J_{i,i+1}^{\alpha}$ with $1 \leqslant i \leqslant N_S - 1$ are set to $J = -1$, and all nonzero $\Omega_{i,j}^{\alpha}$ and $\Delta_{i,j}^{\alpha}$ are randomly generated from the range $[-4/3,4/3]$. Here we present only simulation results for the decoherence measure σ, as the thermalization measure δ behaves similarly. We have included the graphs for δ and b in Appendix A.

1. Different initial states

We first study the decoherence process by solving the TDSE for an entirety at finite temperature starting in two different initial states:

(1) X. The initial state of the entirety $S + E$ is in a canonical-thermal state defined by Eq. (11). The real-time dynamics will not play a significant role in measurements of $\sigma(t)$ and $\delta(t)$ for such an initial state, except for some small fluctuations due to quantum and/or thermal effects. However, for other quantities, for example, expectation values for time-displaced expectation values such as $\langle S_1^z(0)S_1^z(t)\rangle$, the time dependence can be significant.

(2) *UDUDY*. For $N_S = 4$, the initial state of the entirety is a product state of the system and environment. The first four spins (those in S) are in the up, down, up, down state, and the remaining spins (those in E) are in a canonical-thermal state Y.

Quantum dynamics may drive the entirety with arbitrary initial state, including the *UDUDY* state, into a state which is indistinguishable from a state drawn from the ensemble of canonical-thermal states of the entirety. The state observed after sufficiently long times may be expected to resemble a canonical-thermal state X. For an initial state *UDUDY*, the initial temperature of E used to calculate the canonical-thermal state Y will be different from the temperature of the corresponding long-time value of the entirety canonical-thermal state X.

Figure 2 presents the time evolution of $\sigma(t)$ for a spin entirety with $N_S = 4$ and $N_E = 22$ prepared in these two different initial states. For both initial states the inverse temperature is set to $\beta|J| = 0.900$. From Fig. 2, one sees that for the entirety prepared in the product state *UDUDY* $\sigma(t)$ evolves closely to the value obtained for the entirety prepared in the canonical-thermal state X. Of course, the fitting parameter b from Eq. (7) calculated for the initial state *UDUDY* is larger than the initial β for the canonical state X because the initial state of the system is closer to the ground-state energy.

The bottom (green) curve (in both the main figure and the inset of Fig. 2) depicts $\sigma(t)$ for an initial state drawn from X at inverse temperature $\beta|J| = 0.900$ and has an average fitting parameter $b|J| = 0.895$. The inset shows the time average for long times for $\sigma(t)$ for the *UDUDY* initial state with $\beta|J| = 0.900$ (dark khaki curve). The standard deviation of the time average for $t > 300/|J|$ of $\sigma(t)$ for the *UDUDY* initial state is 6×10^{-5}, while the fit to the parameter b from Eq. (7) gives the average $b|J| = 0.926$. The green bottom curve in the inset is the same curve as shown in the main figure, for the initial state X with $\beta|J| = 0.900$. As seen from the inset, the initial states X (green curve) and *UDUDY* (dark khaki curve) lead to different average values for $\sigma(t)$. The final state obtained for the simulation with the *UDUDY* initial state is expected to correspond closely to an X state at a different temperature. Therefore, in the inset we show two other curves for X states with different values of $\beta|J|$. The middle curve (blue) is for an initial state X with $\beta|J| = 0.930$ (giving an average fitting parameter $b|J| = 0.924$). The top curve (red) is for an initial state X with $\beta|J| = 0.945$ (yielding an average fitting parameter $b|J| = 0.939$). Thus, for sufficiently long times, the value of $\sigma(t)$ obtained for the entirety being in the initial *UDUDY* state at a given temperature is well approximated by its value obtained for the entirety being in a state X at a different temperature.

As seen from Fig. 2, the time needed to reach a stationary value for $\sigma(t)$ (with small fluctuations) is quite long for the entirety starting in the *UDUDY* state. For the ring geometry of the entirety used in Fig. 2 there are only two terms in the interaction Hamiltonian H_{SE}. If more terms were added in H_{SE} the relaxation time could be reduced dramatically, as was observed at infinite temperature [39]. There are also cases in which the entirety cannot be driven into a state which is close to the state obtained for the entirety being initially in a canonical-thermal state. For example, at infinite temperature this was observed when conserved quantities other than the total energy or when particular geometric structures were involved [39]. Such exceptional cases are not considered in the present paper.

In principle, high statistics for our measure of decoherence σ for a particular H_S could be obtained from performing four different averages. As seen in Fig. 2, an average over time starting from a particular initial X state could be performed. Another average would be an average over a large number of different initial states, each drawn from the ensemble that gives an X state. In addition to the time average and ensemble average over X states for a fixed environment Hamiltonian H_E, one could also average over different H_E. For each H_E the coupling coefficients $\Omega^{\alpha}_{i,j}$ are randomly generated. One could also average over different Hamiltonians H_{SE} that couple S to E. There is only one realization for H_E used for the results shown in Fig. 2. In order to demonstrate that different realizations of H_E do not significantly affect the values of σ and δ, we present simulation results for σ with different H_E in Fig. 3. For each realization of H_E, a number of different initial states drawn from the ensemble that gives an X state at $\beta|J| = 0.90$ are shown. The average and standard deviation of σ, obtained from all (blue pluses) data points in Fig. 3, are 1.25×10^{-3} and 6.62×10^{-5}, respectively. Figure 3 demonstrates that the value of σ does not differ significantly for different H_E or for different initial X states. For comparison, Fig. 3 also shows the time dependence of σ for the first realization of H_E and one of the initial states X by the green curve, which is the same as the one in Fig. 2. A high-precision calculation for an average value of σ would require taking into account a time average, an ensemble average over initial states X, and an average over different Hamiltonians H_E and λH_{SE} (with fixed D_E and D_S). In this paper we are interested in how σ and δ vary with different values of D_E, D_S, β, and λ. The trends we focus on do not require extremely high-precision measurements. Therefore, we conclude that for our investigation of σ and δ it is sufficient to consider only one realization of H_E and H_{SE} and one realization of the initial X state; averaging over time is not necessarily required.

In the remainder of the paper we focus only on the initial state of the entirety $S + E$ being an X state. In addition, we omit the time index t for the measures of decoherence σ and thermalization δ. For entireties of size $N = N_S + N_E < 32$, the values of σ (δ) are taken from either the time averages or the last time step of $\sigma(t)$. For large system sizes ($N > 32$), it is not necessary to perform real-time simulations as the fluctuations are very small (data not shown).

2. *Coupled spin entirety*

We consider the coupled ring entirety with $\lambda \neq 0$ and investigate how σ behaves with changing global interaction strength λ and inverse temperature β. In all cases we start with an entirety prepared in the canonical-thermal state X and measure σ. The strengths for the two interaction bonds in the Hamiltonian H_{SE} are randomly generated and are kept the same for all considered entireties. Note that H_E is totally different for each realization of the environment with size N_E.

Figure 4 presents simulation results for σ for a fixed system size $N_S = 4$ and different environment sizes N_E. The initial state is prepared at inverse temperature $\beta|J| = 0.90$. From Fig. 4 two regimes with different behaviors of σ as a function of N_E can be observed. The two regimes are separated by a given environment size that depends on the global interaction strength λ and is denoted by $L(\lambda)$. For $N_E < L(\lambda)$, σ decreases approximately exponentially with increasing N_E. For $N_E > L(\lambda)$, σ converges to a finite value that also depends on λ. The smaller is λ, the larger is $L(\lambda)$ and the smaller is the value to which σ converges. We infer from this that σ may not go to zero once H_{SE} is present, that is, once the system and environment are coupled. This would imply that S does not decohere thoroughly even when the size of the environment reaches the thermodynamic limit ($N_E = +\infty$). The inset in Fig. 4 shows σ as a function of λ for $N_E = 36$. It is seen that $\sigma \sim 0.001\lambda^2$. This implies that complete decoherence for S requires both $N_E \to +\infty$ and $\lambda \to 0$. However, numerically we cannot rule out a slow decrease of σ with N_E for finite λ.

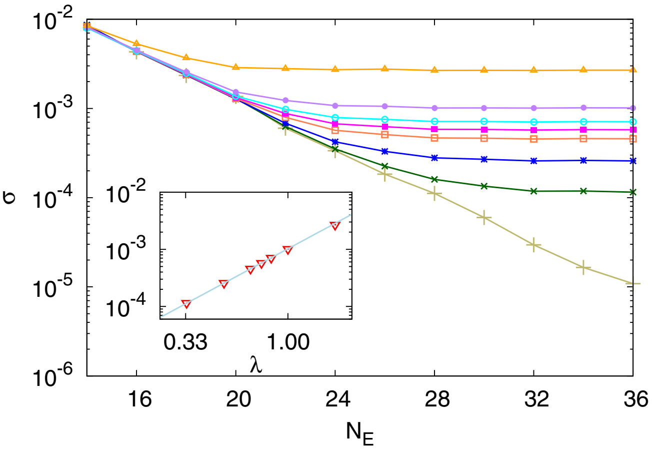

FIG. 4. Simulation results for σ for a coupled ring entirety with $N_S = 4$ and $N_E = 14,\ldots,36$ for different global interaction strengths λ. The entirety is in a canonical-thermal state with $\beta|J| = 0.90$. Curves from bottom to top correspond to $\lambda =$ 0.00, 0.33, 0.50, 0.67, 0.75, 0.83, 1.00, 1.67. (Inset) σ as a function of λ for $N_E = 36$. The (light blue) solid line is a fitting curve for nonzero λ and gives $\sigma \sim 0.001\lambda^2$.

Figure 5 presents simulation results for σ for the coupled ring entirety for different temperatures β. In this case $\lambda = 1$. We observe the same features as for the results shown in Fig. 4 for varying λ. In Fig. 5, σ first decreases approximately exponentially for small N_E and then gradually converges to a finite value for large N_E. The point of crossover shifts to larger N_E for smaller values of β. Although Fig. 5 presents mainly results for finite $\beta|J| < 1$, we observe the same type of curves for finite $\beta|J| \geqslant 1$ (not shown).

In Fig. 5 we also present results for the entirety being in the ground state ($\beta = +\infty$). We used the Lanczos algorithm to obtain the ground state of the entirety $S + E$. The fluctuations of σ for different N_E are large compared to the fluctuations in the results for σ at finite temperature. One cause of this is the unavoidable error made in finding the exact ground state, leading to a different effective inverse temperature β for different N_E. Another cause is that for every value of N_E the bath is completely different, and for each value of N_E we performed the Lanczos calculations for only one particular bath described by the Hamiltonian H_E. Different

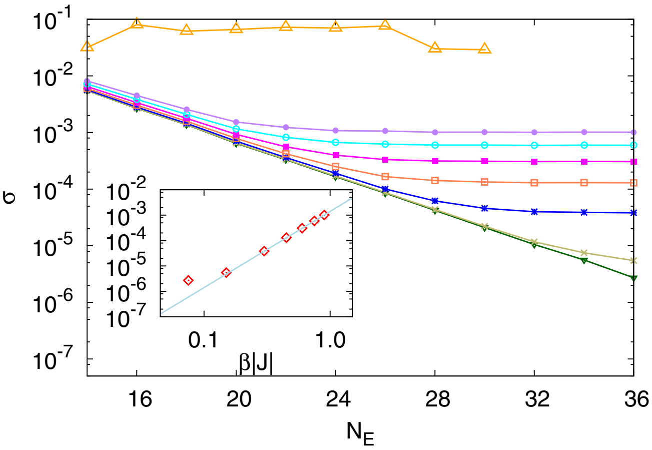

FIG. 5. Simulation results for σ for a coupled ring entirety with $N_S = 4$, $N_E = 14,\ldots,36$, and $\lambda = 1$ for different inverse temperatures β. Curves from bottom to top correspond to $\beta|J| = 0.075, 0.15, 0.30, 0.45, 0.60, 0.75, 0.90, +\infty$. (Inset) σ as a function of $\beta|J|$ for $N_E = 36$. The (light blue) solid line is a fitting curve and gives $\sigma \sim 0.0014\,|J|^3\beta^3$ for $\beta|J| \geqslant 0.15$.

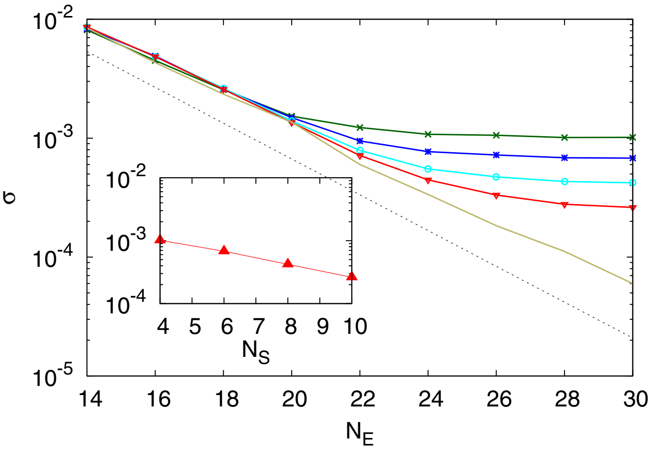

FIG. 6. Simulation results for σ for a coupled ring entirety with $N_S = 4,6,8,10$ (symbols, top to bottom), $N_E = 14,\ldots,30$, and $\lambda = 1$ for $\beta|J| = 0.90$. The solid (dark khaki) line depicts the simulation results for the uncoupled entirety ($\lambda = 0$) with $\beta|J| = 0.90$. The dotted line depicts the analytical results for infinite temperature [39]. (Inset) σ as a function of N_S for $N_E = 30$.

baths [different values of the $\Omega^{\alpha}_{i,j}$ in Eq. (14)] for the same value of N_E may be expected to give very different values for σ, which should be more pronounced for large values of N_E at low temperature. Due to limited computer resources, it was not possible to run the Lanczos algorithm for even larger systems. Within the calculational accuracy and with these caveats, we speculate that σ is flat and converges to a large value at the ground state.

The insets of Figs. 4 and 5 present the results for σ as a function of λ and β, respectively, for $N_E = 36$. At relatively large values of λ and β, σ already approaches its plateau value for $N_E = 36$. The only outlier point is for $\beta|J| = 0.075$ in the inset of Fig. 5. We ignored this point in the fit because from Fig. 5 the asymptotic value for large N_E had not yet been reached for $N = 40$ spins. From these insets we find that the plateau values for σ for large N_E can be fitted well by functions of λ^2 and β^3 for $\lambda < 1$ and $\beta|J| < 1$.

We have previously shown that σ goes to zero in the thermodynamic limit if $\beta = 0$ [39] [see Eq. (8)]. From Figs. 4 and 5, it can be concluded that for large sizes of the environment, σ converges to a value $(\beta\lambda)^2(c_2 + c_3\beta)$ for $0.1 < \beta|J| < 1$ and $0.33 < \lambda < 1$, where the coefficients c_2 and c_3 depend on the specific form of the interaction Hamiltonian H_{SE}, even in the thermodynamic limit. The presence of finite interactions between the system and the environment results in the system not decohering thoroughly (σ remains finite) even when the size of the environment goes to infinity ($D_E \to +\infty$). In order to retrieve $\sigma \to 0$ in the thermodynamic limit ($D_E \to +\infty$), one might have to go simultaneously to the weak-interaction region. Hence, complete decoherence of the system with fixed N_S at finite temperature may require a limiting procedure in which λN_E is kept fixed as $N_E \to +\infty$ and $\lambda \to 0$.

All the results shown in Fig. 4 and 5 are for system size $N_S = 4$. In Fig. 6, we present results for different system sizes $N_S = 4,6,8,10$. It is seen that the values of σ converge to a different finite value for different N_S, and this value decreases as N_S increases. Therefore, σ might go to zero if $N_S \to +\infty$ and $N_E \to +\infty$. Effectively, in this limit one enters the weak-interaction regime for a ring geometry because λ is fixed while both N_E and N_S approach infinity.

3. *Uncoupled spin entirety*

As shown in the previous section, one may have $\sigma = 0$ in the thermodynamic limit if λ goes to zero (see Fig. 4). The uncoupled case ($\lambda = 0$) is a special case which we explore further in this section. Even though $\lambda H_{SE} = 0$, the states of the entirety which are drawn from the ensemble of canonical thermal states [see Eq. (11)] are not direct product states. In other words, the states of S and E are entangled even if $\lambda = 0$, because the entirety is prepared in a canonical-thermal state. Figure 7 shows the simulation results of σ for an uncoupled entirety as a function of the size of the environment N_E for a number of values for the inverse temperature β. The value of σ decreases approximately exponentially with the size of the environment.

In Fig. 7 the absolute value of the slope decreases slightly as $\beta|J|$ increases. When $\beta \to +\infty$, the slope of σ becomes zero and the curve is a horizontal line. The entirety stays in the ground state as $\beta \to +\infty$. If the ground state of S is nondegenerate, then $\sigma = 0$, and if the ground state of S is degenerate, then σ is generally finite for $\beta \to +\infty$.

C. Summary of simulation results

Unlike what we found in our previous work for $\beta = 0$ [39], at finite β the behavior of our measure σ for the decoherence of S is quite different. For any finite values of β and λ, σ decreases approximately exponentially with N_E if N_E is smaller than a certain threshold and converges to a finite value for large N_E. This implies that S will not totally decohere even if $N_E \to +\infty$. The numerical results suggest that $\sigma \approx (\beta\lambda)^2(c_2 + c_3\beta)$ for certain ranges of λ and β in the thermodynamic ($N_E \to +\infty$) limit. In order to have $\sigma = 0$ in the thermodynamic

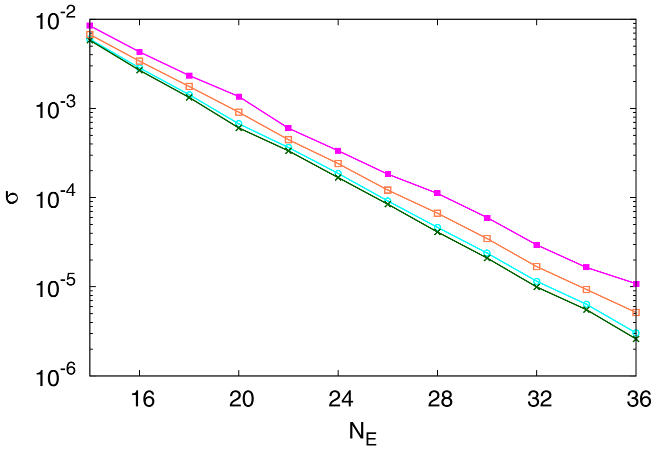

FIG. 7. Simulation results for σ for an uncoupled entirety ($\lambda = 0$) with $N_S = 4$ and $N_E = 14, \ldots, 36$ for different inverse temperatures. Curves from bottom to top correspond to $\beta|J| = 0.075$, 0.30, 0.60, 0.90.

limit, either β goes to zero (our previous results [39]), or λ goes to zero, which is an uncoupled entirety. We emphasize that the uncoupled entirety must be understood as a limiting case of $\lambda \to 0$, since the states of S and E are entangled in a canonical-thermal state X. If one instead directly starts with the initial entirety state being an uncoupled direct product state, then it always will remain a direct product state.

We stress that the calculations presented in this section were extremely expensive to perform in terms of computer resources. Computer memory and CPU time put limitations on the size of the quantum system that can be simulated. The required CPU time is mainly determined by the number of operations to be performed and does not currently put a hard limit on the simulation. However, the memory of the computer does put on a hard limitation. We have studied sizes of the entirety $S + E$ ranging from $N = 18$ to $N = 40$. The largest and most costly simulations were the computations of the decoherence for a $N = 40$ spin-$\frac{1}{2}$ system at various temperatures β and global interaction strengths λ. It took about 1.6×10^6 core hours to complete the eight data points for $N_E = 36$ ($N = 40$) in Fig. 4 on 131 072 processors of JUQUEEN, an IBM Blue Gene/Q located at the Jülich Supercomputer Centre in Jülich Germany [50]. The $N = 40$ points require using 64 TB (terabytes) of memory (SDRAM-DDR3) just to store the four required wave vectors. However, some additional memory is required to store other quantities, making it necessary to run with an allocation of 128 TB spread over the 131 072 processors.

IV. PERTURBATION THEORY

Most of the interesting numerical results in Sec. III are based on an initial state of the type X, which means that the entirety is in a canonical-thermal state. As seen in Figs. 2 and 3, except for small fluctuations the quantum dynamics does not play a significant role for our decoherence measure $\sigma(t)$ [nor does it play a significant role for $\delta(t)$]. Therefore, we again leave the time index t from our expressions for σ and δ. This allows us to perform certain analytical calculations dealing only with the imaginary-time propagation $\exp(-\beta H/2)$ of Eq. (11), which we do here. The derivations are long, and hence only the sketch of the calculations and the final results are presented in the main text. The long derivations are relegated to Appendix B. Especially for the uncoupled entirety $S + E$ ($\lambda = 0$), we are able to derive closed forms for the measures of decoherence and thermalization, namely σ and δ. It is important to remember that even when $\lambda = 0$ the state of the entirety is not a direct product state of states of S and E. These closed forms for σ and δ may be useful for understanding and making predictions of physical systems in certain circumstances. For the coupled case, we derive the first-order perturbation term in the global interaction strength λ and show that the first-order term is exactly zero if the system obeys a certain common symmetry introduced below. The vanishing of the first-order term in λ means that the results of the closed expressions for the uncoupled entirety fit extremely well results for the coupled entirety at small values of $\lambda\beta$.

Hereafter, we investigate the properties of the decoherence measure σ of a quantum system S when the entirety $S + E$ is in the canonical-thermal state [see Eq. (11)]. In essence, our calculations average over the entire ensemble of canonical-thermal states X for a fixed β for any entirety Hamiltonian H.

A. Canonical-thermal state

In the eigenenergy basis $\{|E_k\rangle\}$ of the Hamiltonian H of the entirety, the state of Eq. (11) is given by

$$|\Psi_\beta\rangle = \sum_{k=1}^{D} \frac{d_k e^{-\beta E_k/2}}{\sqrt{\sum_{k'=1}^{D} |d_{k'}|^2 e^{-\beta E_{k'}}}} |E_k\rangle = \sum_{k=1}^{D} a_k |E_k\rangle, \quad (16)$$

where a_k is given by

$$a_k = \frac{d_k p_k^{1/2}}{\sqrt{\sum_{k'=1}^{D} |d_{k'}|^2 p_{k'}}}, \quad (17)$$

$$p_k = \frac{e^{-\beta E_k}}{\sum_{k'=1}^{D} e^{-\beta E_{k'}}}. \quad (18)$$

Note that, in general, the probability density of the coefficient a_k is not Gaussian anymore, as it was at infinite temperature. The $\{a_k\}$ satisfy the required normalization condition, $\sum_{k=1}^{D} |a_k|^2 = 1$. For sufficiently large D (the dimension of the entirety), we have [41]

$$\sum_{k=1}^{D} |d_k|^2 p_k \approx \frac{1}{D}. \quad (19)$$

Equation (19) is a good approximation for all values of λ and β (see Fig. 23 in Appendix B); in fact, Eq. (19) is exact both for $\beta = 0$ and $\beta = \infty$. Therefore, the canonical-thermal state can be written to a good approximation as

$$|\Psi_\beta\rangle = D^{1/2} \sum_{k=1}^{D} d_k p_k^{1/2} |E_k\rangle. \quad (20)$$

B. Uncoupled entirety with Eq. (20) approximation

First we consider an uncoupled entirety with $H_{SE} = 0$ or $\lambda = 0$. There exist simple relations for the eigenvalues

E_k (eigenstates $|E_k\rangle$) of the entirety Hamiltonian H in terms of the eigenvalues $E_i^{(S)}$ and $E_p^{(E)}$ (eigenstates $|E_i^{(S)}\rangle$ and $|E_p^{(E)}\rangle$) of the system Hamiltonian H_S and environment Hamiltonian H_E, respectively, i.e., $E_k = E_i^{(S)} + E_p^{(E)}$ and $|E_k\rangle = |E_i^{(S)}\rangle|E_p^{(E)}\rangle$. The canonical-thermal state reads [from the Eq. (20) approximation]

$$|\Psi_\beta\rangle = D^{1/2}\sum_{i=1}^{D_S}\sum_{p=1}^{D_E} d_{i,p}\,p_{i,p}^{1/2}\big|E_i^{(S)}\big\rangle\big|E_p^{(E)}\big\rangle. \tag{21}$$

The matrix element (i,j) of the reduced density matrix of S, in the basis that diagonalizes H_S, is given by

$$\widetilde{\rho}_{ij} = \mathrm{Tr}_E|\Psi_\beta\rangle\langle\Psi_\beta| = D\sum_{p=1}^{D_E} d_{i,p}^* p_{i,p}^{1/2} d_{j,p}\,p_{j,p}^{1/2}. \tag{22}$$

The expectation value of the off-diagonal matrix elements $(i \neq j)$ with respect to the probability distribution of the random variables $d_{i,p}$ is given by [39,40]

$$\begin{aligned}
\mathscr{E}(2\sigma^2) &= \mathscr{E}\left(\sum_{i\neq j}^{D_S}\left|D\sum_{p=1}^{D_E} d_{i,p}^* p_{i,p}^{1/2} d_{j,p}\,p_{j,p}^{1/2}\right|^2\right)\\
&= D^2\sum_{i\neq j}^{D_S}\sum_{p=1,p'=1}^{D_E}\mathscr{E}(d_{i,p}^* d_{j,p} d_{i,p'} d_{j,p'}^*)\,p_{i,p}^{1/2}p_{j,p}^{1/2}p_{i,p'}^{1/2}p_{j,p'}^{1/2}\\
&= D^2\sum_{i\neq j}^{D_S}\sum_{p=1}^{D_E}\mathscr{E}(|d_{i,p}|^2|d_{j,p}|^2)\,p_{i,p}\,p_{j,p}\\
&= D^2\mathscr{E}(|d_{i,p}|^2|d_{j,p}|^2)\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\frac{Z_E(2\beta)}{Z_E^2(\beta)},
\end{aligned} \tag{23}$$

where $Z_S(n\beta) = \sum_i e^{-n\beta E_i^{(S)}}$ and $Z_E(n\beta) = \sum_p e^{-n\beta E_p^{(E)}}$ denote the partition functions of the system S and the environment E at inverse temperature $n\beta$, respectively. Here and in the following $\mathscr{E}(\cdot)$ denotes the expectation value with respect to the probability distribution of the random numbers $\{d_{i,p}\}$. We change from the partition function to the free energy

$$Z(n\beta) = \sum_k e^{-n\beta E_k} = e^{-n\beta F(n\beta)}, \tag{24}$$

where $F(n\beta) = -(n\beta)^{-1}\ln Z(n\beta)$, for either the entirety (no subscript), the system with subscript S, or the environment with subscript E. We have

$$\begin{aligned}
\mathscr{E}(\sigma^2) &= \frac{D^2}{2}\mathscr{E}(|d_{i,p}|^2|d_{j,p}|^2)\\
&\quad\times(1-e^{-2\beta[F_S(2\beta)-F_S(\beta)]})e^{-2\beta[F_E(2\beta)-F_E(\beta)]}\\
&= \frac{D}{2(D+1)}(1-e^{-2\beta[F_S(2\beta)-F_S(\beta)]})\\
&\quad\times e^{-2\beta[F_E(2\beta)-F_E(\beta)]},
\end{aligned} \tag{25}$$

where $\mathscr{E}(|d_{i,p}|^2|d_{j,p}|^2) = 1/D(D+1)$ [40]. From Eq. (25), we see that σ scales with the size of the environment for the uncoupled entirety because the free energy F_E scales with the size of the environment. Hence, σ goes to zero in the thermodynamic limit ($N_E \to +\infty$) for this uncoupled case.

For δ, we obtain the expression

$$\mathscr{E}(\delta^2) = \frac{D}{D+1}e^{-2\beta[F_S(2\beta)-F_S(\beta)]}\left(e^{-2\beta[F_E(2\beta)-F_E(\beta)]}-\frac{1}{D}\right) \tag{26}$$

from a similar analysis.

C. Uncoupled entirety with full $|\Psi_\beta\rangle$

These expressions Eqs. (25) and (26) only work for very high or very low temperatures where the approximation in Eq. (20) is valid. The reason is that the derivation of Eqs. (25) and (26) is based on an approximate expression of the canonical-thermal state [see Eq. (21)] by using Eq. (19). In order to improve the above results, we have to perform calculations which start from the canonical-thermal state in Eq. (11). We perform a Taylor series expansion of σ^2 up to second order in $|d|^2$ about the value $1/D$ and then calculate the expectation value of σ^2. A very lengthy calculation, relegated to Appendix B, gives

$$\begin{aligned}
\mathscr{E}(\sigma^2) &= \frac{1}{2}e^{-2\beta[F_E(2\beta)-F_E(\beta)]}(1-e^{-2\beta[F_S(2\beta)-F_S(\beta)]})\\
&\quad-\frac{2D}{D+1}e^{-3\beta[F_E(3\beta)-F_E(\beta)]}\\
&\quad\times(e^{-2\beta[F_S(2\beta)-F_S(\beta)]}-e^{-3\beta[F_S(3\beta)-F_S(\beta)]})\\
&\quad+\frac{3D}{2(D+1)}e^{-4\beta[F_E(2\beta)-F_E(\beta)]}e^{-2\beta[F_S(2\beta)-F_S(\beta)]}\\
&\quad\times(1-e^{-2\beta[F_S(2\beta)-F_S(\beta)]}).
\end{aligned} \tag{27}$$

Obviously, in most cases the first term will dominate, which approaches Eq. (25) for D large.

Two special cases are of interest. If $\beta = 0$, we recover the previous result $\mathscr{E}(\sigma^2) = \frac{D_S-1}{2(D+1)}$ [39]. In the vicinity of $\beta = 0$, the first-order term of the Taylor expansion of Eq. (27) vanishes. Hence, in the high-temperature limit, $\mathscr{E}(\sigma^2) = \frac{D_S-1}{2(D+1)} + \mathscr{O}(\beta^2)$.

If the temperature approaches zero, Eq. (27) becomes

$$\lim_{\beta\to+\infty}\mathscr{E}(\sigma^2) = \frac{g_S-1}{2g_Sg_E}\left[1-\frac{D_SD_E}{(D_SD_E+1)g_Sg_E}\right], \tag{28}$$

where g_S and g_E refer to the degeneracy of the ground state of the system S and environment E, respectively. This expression yields zero if the ground state of the system is nondegenerate. For a system with a highly degenerate ground state ($g_S \gg 1$), the expression goes to $1/2g_E$. For a system with known $g_S > 1$ and a large environment $D_E \gg 1$, at small λ and at low temperature, if one measures $\mathscr{E}(\sigma^2)$, one can determine the degeneracy g_E of the ground state of the environment. This is a new, strong prediction. The ground-state degeneracy g_E of the environment can be obtained by only measuring quantities in the system S.

Similarly, we can make the Taylor expansion for δ^2 up to second order with respect to both $|d|^2$ and b about the values $1/D$ and β, respectively. The full derivation is given in Appendix B. The expectation value of δ^2 is given by

$$\begin{aligned}
\mathscr{E}(\delta^2) &= \frac{D}{D+1}e^{-2\beta[F_E(2\beta)-F_E(\beta)]}(e^{-2\beta[F_S(2\beta)-F_S(\beta)]}\\
&\quad-2e^{-3\beta[F_S(3\beta)-F_S(\beta)]}+e^{-4\beta[F_S(2\beta)-F_S(\beta)]})\\
&\quad+e^{-2\beta[F_S(2\beta)-F_S(\beta)]}\{[C_S(2\beta)/(4\beta^2)]\\
&\quad+[U_S(2\beta)-U_S(\beta)]^2\}(\Delta b)^2,
\end{aligned} \tag{29}$$

where $\Delta b = b - \beta$, and $C_S(n\beta)$ and $U_S(n\beta)$ are, respectively, the specific heat and average energy of the system S at inverse temperature $n\beta$. It is obvious that for the uncoupled entirety $b = \beta$. For the coupled entirety, as we find below, b is not necessarily equal to β, but should usually be close to the value of β.

D. Coupled entirety

For a generic entirety, a system S is coupled to an environment E. To solve such a coupled entirety analytically, we have to resort to a perturbation theory. Up to first order in the global system-environment coupling strength λ, we have [51]

$$e^{-\beta H} \approx \left(1 - \left\{\int_0^1 d\xi e^{-\beta\xi H_0} H_{SE} e^{\beta\xi H_0}\right\}\beta\lambda\right)e^{-\beta H_0}, \quad (30)$$

where $H_0 = H_S + H_E$ denotes the Hamiltonian of the uncoupled system and environment.

The first-order perturbation comes from both the denominator and numerator of Eq. (11). First let us deal with the denominator. Up to the first order, we have

$$\begin{aligned} &D\langle\Psi(0)|e^{-\beta H}|\Psi(0)\rangle \\ &\quad\approx \mathrm{Tr}e^{-\beta H_0} - \beta\lambda\int_0^1 d\xi \mathrm{Tr}e^{-\beta\xi H_0} H_{SE} e^{-\beta(1-\xi)H_0}. \end{aligned} \quad (31)$$

Hereafter, we introduce a kind of symmetry which makes the first-order term in Eq. (31) be zero and restrict ourselves to a system which obeys such a symmetry. The symmetry is a kind of unitary transformation such that if we reverse the components in the system S or in the environment E, the sign of the interaction Hamilton H_{SE} is reversed while the Hamiltonians H_S and H_E are unchanged. Let Z_0 be the partition function of the unperturbed system (the uncoupled entirety where $H_{SE} = 0$). The complete symmetry requirement can easily be seen by performing the integration over ξ in Eq. (31) to give

$$D\langle\Psi(0)|e^{-\beta H}|\Psi(0)\rangle \approx Z_0 - \beta\lambda \mathrm{Tr}_{S,E}(H_{SE}e^{-\beta H_E}e^{-\beta H_S}) \quad (32)$$

and asking when the trace that multiplies $\beta\lambda$ vanishes. With such a symmetry involved, it is clear that the first-order term in Eq. (31) has to be zero. Then the first-order perturbation term can only come from the numerator of Eq. (11).

Consequently, up to the first order, we have

$$\langle\Psi(0)|e^{-\beta H}|\Psi(0)\rangle \approx \mathrm{Tr}e^{-\beta H_0}/D = Z_0/D. \quad (33)$$

The wave function is thus given approximately by

$$\begin{aligned} |\Psi_\beta\rangle &\approx \sqrt{\frac{D}{Z_0}}\, e^{-\beta H/2}|\Psi(0)\rangle \\ &\approx \sqrt{\frac{D}{Z_0}}\left(1 - \left\{\int_0^1 d\xi e^{-\beta\xi H_0/2} H_{SE} e^{\beta\xi H_0/2}\right\}\beta\lambda/2\right) \\ &\quad\times e^{-\beta H_0/2}|\Psi(0)\rangle. \end{aligned} \quad (34)$$

Based on the expression in Eq. (34), we find that the first-order term of the perturbation expansion in λ of the expectation value of σ^2 is given by

$$\begin{aligned} \mathscr{O}(\mathscr{E}(\sigma^2))_{\lambda^1} &= -\beta\lambda\left(\frac{D}{Z_0}\right)^2 \frac{D}{D+1} \\ &\quad\times [Z_S \mathrm{Tr}e^{-\beta H_S} e^{-2\beta H_E} H_{SE} - \mathrm{Tr}e^{-2\beta(H_S+H_E)} H_{SE}]. \end{aligned} \quad (35)$$

Applying the same symmetry transformation as discussed before results in $\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} = 0$. In other words, the same symmetry that makes the $\beta\lambda$ term in Eq. (32) zero will make both traces in Eq. (35) zero. Hence, to study the decoherence of a system S coupled to an environment E up to first order in λ, it is *sufficient to study the uncoupled entirety* ($\lambda = 0$) (see the results in Sec. IV C).

Calculating the second-order perturbation term of σ^2 is much more complicated as the perturbation term comes from both the denominator and numerator of Eq. (11). In terms of perturbation theory, the reduced density matrix of S can be written as

$$\begin{aligned} \widetilde{\rho} &= \frac{\mathrm{Tr}_E e^{-\beta H/2}|\Psi(0)\rangle\langle\Psi(0)|e^{-\beta H/2}}{\langle\Psi(0)|e^{-\beta H}|\Psi(0)\rangle} \\ &= \widetilde{\rho}_0 + \beta\lambda\widetilde{\rho}_1 + (\beta\lambda)^2\widetilde{\rho}_2 + \cdots, \end{aligned} \quad (36)$$

where $\widetilde{\rho}_0$ is the zeroth-order term which represents the reduced density matrix of the uncoupled entirety ($\lambda = 0$), and $\widetilde{\rho}_1$ and $\widetilde{\rho}_2$ are matrices representing the first- and second-order perturbation terms. We have shown that $\widetilde{\rho}_1 = 0$ if the Hamiltonian of the entirety has the previously discussed symmetry. If $\widetilde{\rho}_2$ or higher-order terms are nonzero, then σ will be finite at finite λ. If $\beta\lambda \ll 1$, we can safely use the results obtained from the uncoupled entirety for the measures of decoherence and thermalization. It is important to remember that the initial state of the uncoupled entirety ($\lambda = 0$) is not a direct product state of states of S and E.

E. Verification by spin Hamiltonians

From Eqs. (13)–(15) it is seen that the Hamiltonian of the spin entirety obeys the symmetry property required to make the first-order term λ^1 of the perturbation expansion of the expectation value of σ^2 [see Eq. (35)] exactly zero. Namely, reversing all spin components of the system or of the environment spins does not change H_S or H_E, but the sign of H_{SE} changes. Note that such a symmetry is also obeyed in the case where there is no interaction between the environment spins, e.g., for an environment Hamiltonian $H_E = -\sum_{i=1}^{N_E}\sum_{\alpha=x,y,z} h_i^\alpha I_i^\alpha$ [52,53]. In this particular case, it is only required that H_S is an even function and H_{SE} an odd function under reversal of all spin components of the system spins.

For a small size of the system such as $N \leqslant 12$, we can diagonalize the system exactly, find all the eigenvalues and eigenstates of the Hamiltonians H_S and H_E, and directly calculate the values of σ and δ according to the analytical expression of Eqs. (27) and (29), respectively.

Figure 8 shows the simulation results for $\sqrt{\mathscr{E}(\sigma^2)}$ obtained by exact diagonalization for the entirety $S + E$ being a spin chain with $N_S = 4$ and $N_E = 8$. The system S and environment E consist of two ferromagnetic spin chains with isotropic spin-spin interaction strengths $J_{i,j}^\alpha = J = \Omega_{i,j}^\alpha = \Omega = 1$. They are connected by one of their end spins,

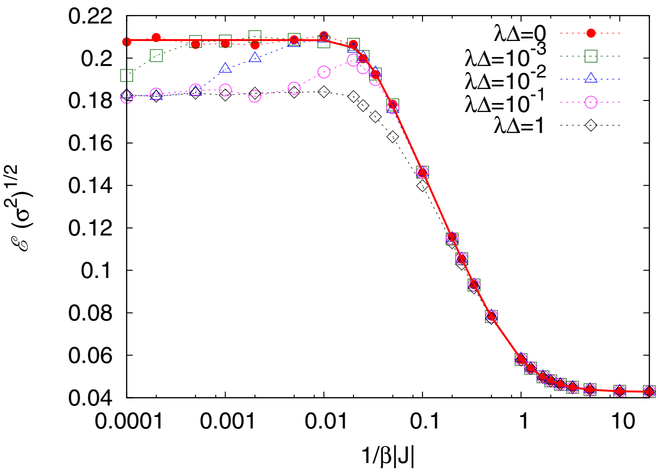

FIG. 8. Simulation results for $\sqrt{\mathscr{E}(\sigma^2)}$ for ferromagnetic spin-$\frac{1}{2}$ chains with $N_S = 4$, $N_E = 8$, $J = \Omega = 1$, and various interaction strengths $\lambda\Delta$ as a function of the temperature $T/J = 1/(\beta J)$. The solid line (red) is obtained from Eq. (27) by using numerical values for the free energies $F_S(n\beta)$ and $F_E(n\beta)$. The dotted lines are guides for the eye.

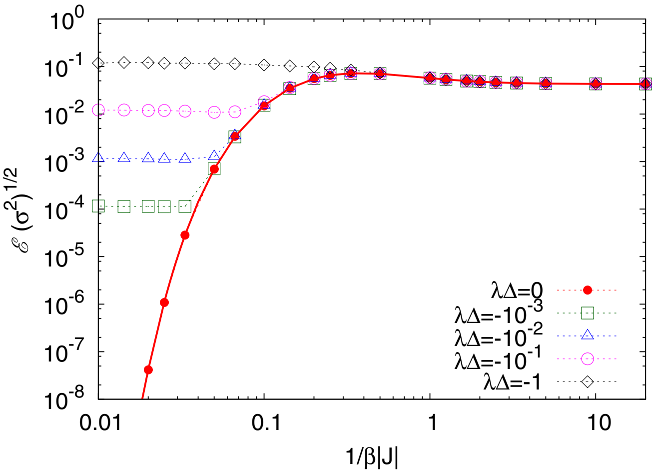

FIG. 9. Simulation results for $\sqrt{\mathscr{E}(\sigma^2)}$ for spin-$\frac{1}{2}$ chains with $N_S = 4$, $N_E = 8$, $J = -1$, $\Omega = 1$, and various interaction strengths $\lambda\Delta$ as a function of temperature $T/|J| = 1/\beta|J|$. The solid line (red) is obtained from Eq. (27) by using numerical values for the free energies $F_S(n\beta)$ and $F_E(n\beta)$. The dotted lines are guides for the eye. Note that this figure is for $g_S = 1$, which looks very different compared to Fig. 8 for $g_S > 1$.

with an interaction strength $\Delta^{\alpha}_{N_S,1} = \Delta$. The global system-environment coupling strength is $\lambda = 1$. The simulation results (symbols) are averages over 1000 simulations with different initial random state vectors drawn from the ensemble X. Substituting the numerically obtained values for the free energy of the system and environment for $\lambda\Delta = 0$ in the analytical expressions for $\mathscr{E}(\sigma^2)$ given by Eq. (27) results in the solid lines depicted in Fig. 8. The simulation results for the uncoupled entirety ($\lambda\Delta = 0$) and for the coupled cases when $\beta\lambda\Delta \leqslant 1$ agree with the analytical results for the whole range of temperatures. As the temperature decreases the state of the entirety $S + E$ approaches the ground state, and $\mathscr{E}(\sigma^2)$ becomes constant, with its numerical value being given by Eq. (28). For the case at hand, $g_S = 5$, $g_E = 9$, $D_S = 16$, and $D_E = 256$; hence, Eq. (28) yields $\sqrt{\mathscr{E}(\sigma^2)} = 0.21$, in excellent agreement with the numerical data. In the coupled case and for small temperatures $1/\beta J$, $\sqrt{\mathscr{E}(\sigma^2)}$ develops a plateau different from that of the uncoupled case. The dependence of this plateau on β or $\lambda\Delta$ is nontrivial, requiring a detailed analysis of how the ground state of $S + E$ leads to the reduced density matrix of S (in the basis that diagonalizes H_S). In this respect, the β or $\lambda\Delta$ dependence of the data shown in Fig. 8 is somewhat special because the ferromagnetic ground state of the system does not depend on $\lambda\Delta$.

For the spin system under study with $\lambda\Delta \neq 0$, the first-order term of the perturbation expansion of the expectation value of σ^2 in terms of $\beta\lambda\Delta$ is exactly zero. Hence, for a weakly coupled entirety ($\lambda\Delta$ small) deviations from the analytical results [Eq. (27)] obtained for the uncoupled entirety ($\lambda\Delta = 0$) are, as expected, seen *only* in the low-temperature region. The numerical results (symbols) in Fig. 8 are in excellent agreement with the predicted results (solid line, red) as long as $\beta\lambda\Delta$ is small. For a finite $\beta\lambda\Delta$, the plateaus at low temperature may or may not be reached, and therefore the perturbation results may no longer be applicable. The results in Fig. 8 are in amazingly good agreement for all temperatures with the perturbation theory predictions of Eq. (27). The excellent agreement is also seen for low temperatures whenever $\beta\lambda\Delta \leqslant 1$, giving agreement with the expression Eq. (28), wherein the ground-state degeneracy of the environment E enters the measured value of σ in the system S.

In the low-temperature limit for $\mathscr{E}(\sigma^2)$ from Eqs. (28) or (B131) the perturbation expression gives

$$\lim_{\beta\to\infty} \mathscr{E}(\sigma^2) \approx \frac{(g_S - 1)(g_S g_E - 1)}{2 g_S^2 g_E^2}, \tag{37}$$

with the approximation valid for large D. In Fig. 8 results for the approach to the low-temperature limit for one case with $N_S = 4$, $N_E = 8$ and $g_S = 5$, $g_E = 9$. For $g_S > 1$ the expression in Eq. (37) is finite at $T = 0$. However, when $g_S = 1$ the expression in Eq. (37) is zero at $T = 0$. Therefore, the predicted curve looks much different from the curve in Fig. 8.

Therefore, we here present results for a case with $g_S = 1$. The system is a spin chain with $N_S = 4$ and isotropic antiferromagnetic spin-spin interactions $J^{\alpha} = -1$ with $\alpha = x,y,z$, so $g_S = 1$. The environment is a spin chain with $N_E = 8$ and isotropic ferromagnetic spin-spin interactions $\Omega^{\alpha} = 1$. The environment and system are connected by one of their end spins to form the entirety $S + E$ with a chain geometry. The coupling interactions $\lambda\Delta^{\alpha}$ take various isotropic values. Figure 9 for $g_S = 1$ looks completely different compared to Fig. 8 for $g_S > 1$. Nevertheless, as the system-environment coupling strength $\lambda\Delta$ becomes small, the data from the calculations fall nicely on the theoretical curve obtained from Eq. (27) (red solid line). Note the extremely small values for $\sqrt{\mathscr{E}(\sigma^2)}$ for low temperatures. Calculating the theoretical curves (red solid lines) for these quantities at low temperatures required quadruple precision in the floating point numbers.

In order to study the behavior of σ as a function of the global coupling interaction strength λ, we performed further simulations for a spin entirety configured as a ring with $N_S = 4$

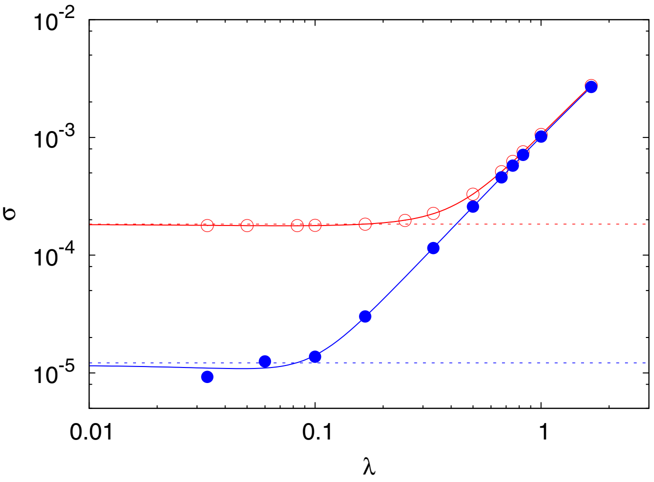

FIG. 10. Simulation results for σ for rings with $N_S = 4$, $N_E = 26$ (open circles) and $N_S = 4$, $N_E = 36$ (solid circles) as a function of the global interaction strength λ for $\beta|J| = 0.90$. For the values of the interaction parameters, see text. The solid lines are fits to the data as described in the text. The top (bottom) horizontal dashed line represents the value obtained by simulating the noninteraction system, $\lambda = 0$, with 30 (40) spins.

and $N_E = 26,36$ at the inverse temperature $\beta|J| = 0.90$. In Fig. 10 we present the simulation results for σ as a function of λ. The entirety is a ring, and the system Hamiltonian H_S is antiferromagnetic (the Hamiltonians and geometry have the same structure as in Figs. 2 through 7). Least-squares fitting of the data for σ^2 to polynomials in λ, we find that a polynomial of degree 7 yields the best fit, for both the 30- and 40-spin entirety data [54,55]. The behavior of δ is very similar to that of σ and is again only shown in Appendix A. From Fig. 10 it is seen that for $\lambda \approx 1$, σ changes very little as the dimension of the Hilbert space of the environment increases. This is a pronounced finite-temperature effect, as for $\beta = 0$ the scaling $\sigma \sim 1/\sqrt{D_E}$ holds independent of the coupling λ [39].

V. CONCLUSIONS AND DISCUSSION

In this paper, we investigated measures σ for the decoherence and δ for the thermalization of a quantum system S coupled to a quantum environment E at finite temperature. The entirety $S + E$ is a closed quantum system of which the time evolution is governed by the TDSE.

Today many technologies are being driven by necessity to the quantum regime, rather than operating in a classical or semiclassical regime. In the quantum regime, maintaining the coherence of the state of the system under investigation is paramount. Therefore, an understanding and quantitative predictions of how difficult it is for a quantum system S to decohere, and how effective a particular quantum environment E is at decohering any system is critical to quantum technologies and experiments such as gate-based quantum computers [23,24], adiabatic quantum computers [25–27], quantum dots [30,31], quantum optics [35], cold atoms [32–34], coherent electron transport [28,29] (including nanoelectronics [56,57] and quantum dragon nanodevices [58,59]), and atom/cavity systems [36]. We have found that at finite and small $\beta\lambda$, where β denotes the inverse temperature and λ the global system-environment coupling strength [see Eq. (1)], the important quantities to answer these questions about decoherence are the free energy F_S of the system S and the free energy F_E of the environment E. Therefore, experimentally it is important to measure or to estimate F_S and F_E. The lowest order result for σ is given in Eq. (25), with the full result given in Eq. (27). Similar statements hold for the measure of thermalization δ, with the lowest-order result given in Eq. (26) and the full result given in Eq. (29) in terms of the free energies of both S and E.

We have investigated σ and δ at finite temperature both numerically and analytically. Most of the numerical results can be understood within the framework of our analytic results. If the entirety $S + E$ is prepared in a canonical-thermal state, we showed by means of perturbation theory that σ^2, the degree of the decoherence of S, is of the order $\beta^2\lambda^2$. Similar results were found for our measure of thermalization δ^2. Up to the first order in the system-environment interaction we found

$$\sigma^2,\delta^2 \propto \exp\{-2\beta[F_E(2\beta) - F_E(\beta)]\}. \tag{38}$$

A related decoherence result, for a somewhat different context, was found in Ref. [42]. Note that F_E is the environment free energy and, consequently, is an extensive quantity. This provides a measure for how well a weakly coupled specific finite environment can decohere and thermalize a system at an inverse temperature β. A measure for how difficult it is to decohere a quantum system is given by ratios of free energies of the system, as in Eq. (27).

To illustrate the power of our conclusions, one could ask of any bath how effective it is to decohere any system. The simplest bath, one often used in theoretical calculations with spin baths, is a collection of noninteracting environment spins ($H_E = 0$). The partition function is then $Z_E = 2^{N_E}$ and the free energy is $F_E = -N_E \ln(2)/\beta$. From Eq. (38) this gives $\sigma, \delta \propto 2^{-N_E}$ for any temperature β. Even if $H_{SE} = 0$ the decoherence goes as 2^{-N_E}, but one needs to remember that the thermal canonical state of the entirety is not a direct product of states of the system and environment. Other related questions can be raised. For example, for the case where $H_E = -\sum_{i=1}^{N_E}\sum_{\alpha=x,y,z} h_i^\alpha I_i^\alpha$ the partition function is $Z_E = 2^{N_E}\prod_{i=1}^{N_E}\cosh(\beta|h_i|)$. Therefore, it does not matter whether all the environment fields point in the same direction or in random directions in terms of the efficiency of the environment to decohere and thermalize any system. Of course, for the same system S but different h_i for this type of environment the ensemble of canonical-thermal states will be different.

We have obtained a very strong prediction at low temperatures for the decoherence, namely Eq. (28). At very low temperatures and for large dimension of the Hilbert space for the entirety $S + E$ this prediction is

$$\mathscr{E}(\sigma^2) = \frac{(g_S - 1)(g_S g_E - 1)}{2 g_S^2 g_E^2}, \tag{39}$$

with the ground-state degeneracy of S (E) given by g_S (g_E). Equation (39) shows that it is possible to perform measurements only on the system S, but from that extract the ground-state degeneracy of the environment E. The results in Fig. 8 are for $g_S > 1$, and a corresponding graph is shown

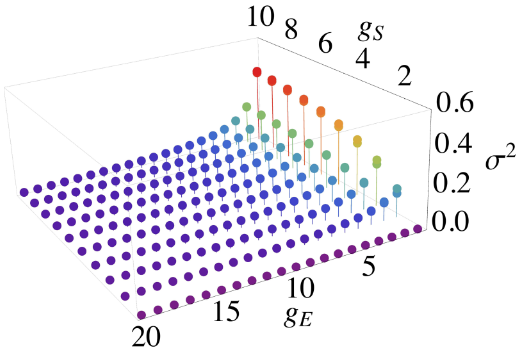

FIG. 11. Predicted results for σ^2 at very low temperatures in terms of the degeneracy g_S of the system and g_E of the environment. These are from Eq. (28). Two values for the dimension D of the Hilbert space of the entirety $S + E$ are plotted, $D = 4$ and $D = 2^{30}$. The difference between these two values of D are only discernible in the case $g_E = 1$.

for a case with $g_S = 1$ in Fig. 9. As predicted by Eq. (39), these two cases look very different in the low-temperature limit. Furthermore, at low temperatures in order for a system to not be able to decohere it is best that the system S has a high degeneracy while the environment E is nondegenerate. This is shown in Fig. 11.

We performed large-scale real- and imaginary-time simulations for N_S spins in the system and N_E spins in the environment. A canonical-thermal state [see Eq. (11)] can be prepared by imaginary-time propagation based on the Chebyshev polynomial algorithm. Starting with such a canonical-thermal state, the simulation results for the uncoupled entirety agree very well with the analytical results (see, in particular, Figs. 8 and 9).

Once the interaction Hamiltonian H_{SE} is turned on, we observe that the decoherence measure σ generally converges to a finite value when the environment size is above a threshold number which depends on the inverse temperature β and the global interaction strength λ (see Figs. 4 and 5). The smaller β and λ are, the larger the threshold number is. When the system size is smaller than the threshold number, σ (and δ) behave as they do for an uncoupled entirety. By an uncoupled entirety we mean that $\lambda H_{SE} = 0$, but the initial state of the system is a canonical-thermal state of the entirety $S + E$ and hence is not a direct product state of states of S and E. After the system size reaches the threshold number, σ (and δ) quickly converges to a finite value, due to the high-order contributions from the interaction H_{SE}. From the numerical simulations, the stationary value of σ has the form $(\beta\lambda)^2(c_2 + c_3\beta)$ for our range of simulation parameters.

Strictly speaking, the system S completely decoheres if there is no interaction between S and E and if $N_E \to \infty$. If S is coupled to E, the H_{SE} interaction is important and both σ and δ are finite for a finite system S even in the thermodynamic limit ($N_E \to +\infty$). However, if the canonical ensemble is a good approximation for the state of the system for some inverse temperatures β up to some chosen maximum energy $E_{\text{hold}} > 0$ (measured from the ground state), then it is required that $\exp(-\beta E_{\text{hold}}) \gg \sigma$. By determining the crossover of the left- and right-side functions, we find a threshold for the temperature above which the state of the system is well approximated by a canonical ensemble and below which quantum coherence of the system is well preserved.

We emphasize that the entirety $S + E$ is initially prepared in a pure state given by a particular choice of a canonical-thermal state X in Eq. (11). With such a state as the initial state for the TDSE, the real-time dynamics does not have much effect on our measures for decoherence (σ) or thermalization (δ). If we start with a nonequilibrium state, such as a product state of S and E, where S is in the ground state and E is in a canonical-thermal state, the real-time dynamics plays an important role in both the decoherence and the thermalization of S [39,41,60], as seen in Fig. 2. At infinite temperature there may exist certain geometric structures or conserved quantities which prevent the system from having complete decoherence [39]. In contrast to the infinite-temperature results, we have found here that at finite temperature the lack of complete decoherence is the normal scenario for any coupled entirety (finite λH_{SE}).

In this paper we have answered important questions about how easily a given system S can decohere or thermalize, and how efficient a given bath is to decohere or thermalize any system. We have not addressed the equally important question of how quickly S thermalizes or decoheres. Nevertheless, we believe that our methodology of simulations and perturbation calculations with thermal canonical states can also be important to address the time-dependent question. For full time dependence, the real-time version of Eq. (30) would need to be used, most likely leading to even more complicated perturbation theory calculations than are detailed in Appendix B.

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APPENDIX A: NUMERICAL RESULTS FOR δ

In the main text, we only present the simulation results for $\sigma(t)$, a measure of the decoherence of a quantum S under the influence of a quantum environment E. The simulation results for $\delta(t)$, a measure of the thermalization of S, given by Eq. (6), are shown in this appendix. The largest entireties we were able to study contained 40 spins, as it requires about 10^{12} floating-point numbers to represent a vector of the Hilbert space of an entirety with this size. A sketch of the ring geometry for $N = 40$ and $N_S = 4$ is given in Fig. 1. We will see that besides the size of the statistical fluctuations, $\delta(t)$ (or the time-independent average δ) behaves very similarly compared to $\sigma(t)$ (or the time-independent average σ). For a single run with

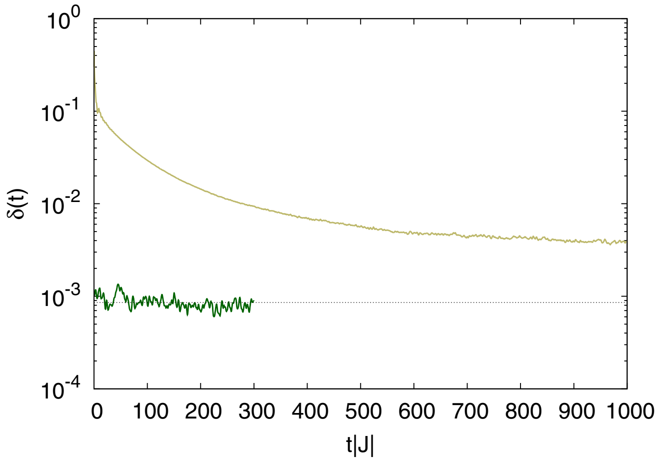

FIG. 12. Simulation results for $\delta(t)$ for a coupled ring entirety with $N_S = 4$, $N_E = 22$, and $\lambda = 1$ for two different initial states X (flat curve, green) and $UDUDY$ (decay curve, dark khaki), with $\beta|J| = 0.90$. The dotted (green) horizontal line is a guide for the eye. This figure corresponds to Fig. 2 in the main text.

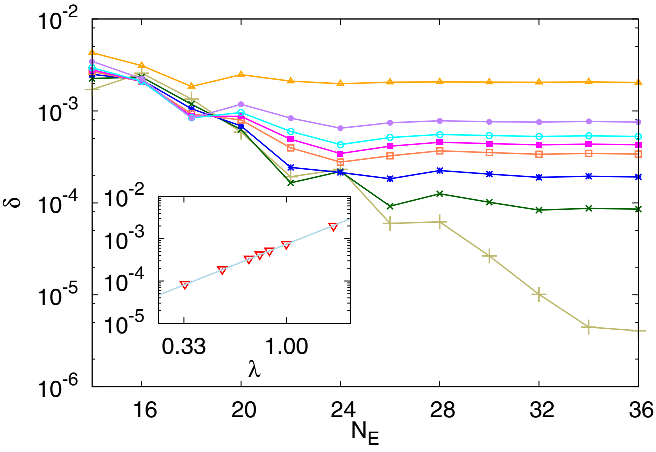

FIG. 14. Simulation results for δ for a coupled ring entirety with $N_S = 4$ and $N_E = 14, \ldots, 36$ for different global interaction strengths λ. The entirety is in a thermal canonical state with $\beta|J| = 0.90$. Curves from bottom to top correspond to $\lambda = 0.00$, 0.33, 0.50, 0.67, 0.75, 0.83, 1.00, 1.67. (Inset) δ as a function of λ for $N_E = 36$. The (light blue) solid line is a fitting curve for nonzero λ and gives $\delta \approx 0.000\,74\lambda^2$. This figure corresponds to Fig. 4 for σ.

one realization of H_E and one representation of the canonical-thermal state [see Eq. (11)], it is obvious that the data for $\delta(t)$ may have stronger statistical fluctuations than those for $\sigma(t)$ shown in the main text, as the number of diagonal elements of the reduced density matrix of the system S are much smaller than the number of the off-diagonal elements.

Figure 12 presents the time evolution of $\delta(t)$ for a spin system with $N_S = 4$ and $N_E = 22$ prepared in two different initial states X and $UDUDY$. From Fig. 12, one sees that $\delta(t)$ obtained from $UDUDY$ evolves closely to the value obtained from X, which is very similar to the behavior of $\sigma(t)$ shown in Fig. 2. The difference of the values of $\delta(t)$ between these two initial states at long times is about 0.003. This difference is larger than that for $\sigma(t)$ at long times. The reason is that the diagonal elements of the reduced density matrix $\widetilde{\rho}$ for S keep a strong memory of the initial state. The memory effects would be reduced for a larger system S.

Figure 13 presents the corresponding results for δ as in Fig. 3 for σ. The average and the standard deviation of the data points shown in Fig. 13 are 8.0×10^{-4} and 1.4×10^{-4}, respectively. As is the case for σ in the main text, the time average for δ and the average over different environment Hamiltonians H_E and different representations of the initial state X all behave similarly.

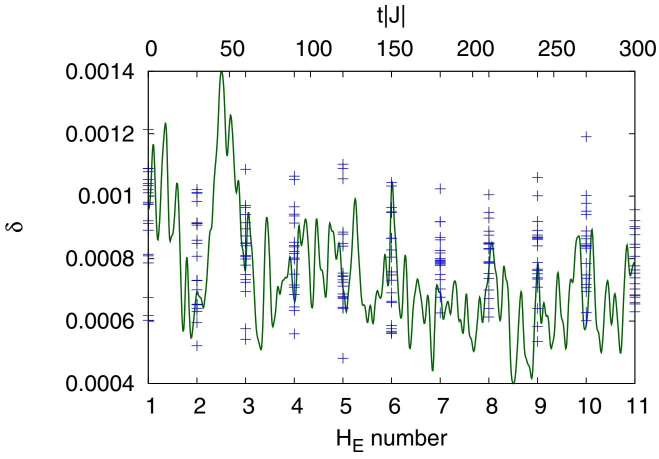

FIG. 13. Simulation results for δ for a coupled ring entirety with $N_S = 4$, $N_E = 22$, and $\lambda = 1$ starting from different initial states X with $\beta|J| = 0.90$. Results for 11 different realizations of the environment Hamiltonian H_E are shown (x-axis label at the bottom), each with different initial states drawn from the ensemble that gives an X state (blue pluses). The time dependence of δ for the first realization of H_E and one of the initial states X is shown by the solid (green) curve (x-axis label on top), which is the same (green) curve depicted in Fig. 12. This figure corresponds to Fig. 3 in the main text.

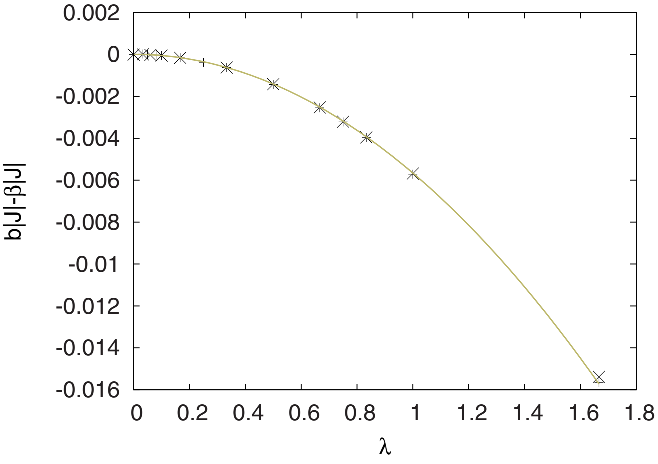

FIG. 15. Simulation results, corresponding to Fig. 14 for the difference between the fitting temperature b and the inverse temperature β for entireties with $N_E = 26$ (pluses) and $N_E = 36$ (crosses). For $\lambda < 1$, the data points fit very well to the curve $b|J| - \beta|J| \approx -0.005\,66\lambda^2$ (solid curve).

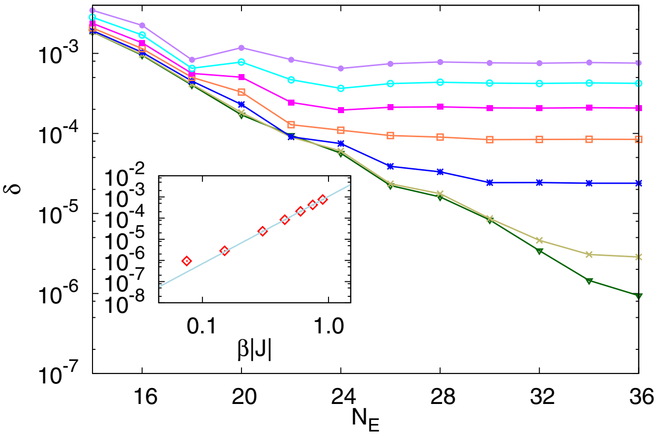

FIG. 16. Simulation results for δ for a coupled ring entirety with $N_S = 4$, $N_E = 14,\ldots,36$, and $\lambda = 1$ for different inverse temperatures β. The initial states are canonical-thermal states at different value of β, corresponding to curves from bottom to top with $\beta|J| = 0.075$, 0.15, 0.30, 0.45, 0.60, 0.75, 0.90. (Inset) δ as a function of $\beta|J|$ for $N_E = 36$. The (light blue) solid line is a fitting curve and gives $\delta \approx 0.001\,06(\beta|J|)^{3.18}$ for $\beta|J| \geqslant 0.15$. This figure corresponds to Fig. 5 in the main text.

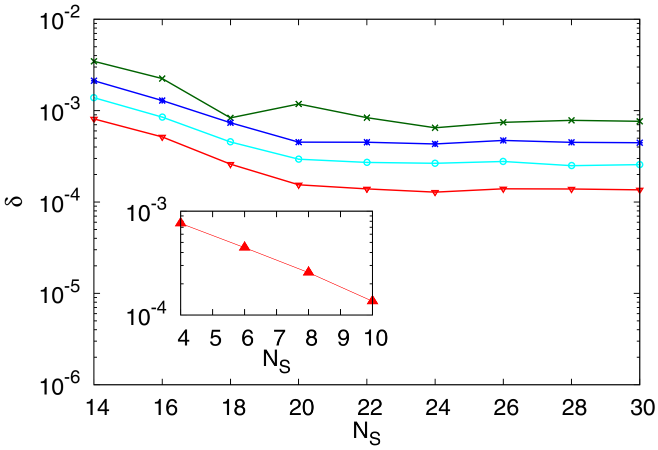

FIG. 18. Simulation results for δ for a coupled ring entirety with $N_S = 4$, 6, 8, 10 (symbols, top to bottom), $N_E = 14,\ldots,30$, and $\lambda = 1$ for $\beta|J| = 0.90$. (Inset) δ as a function of N_S for $N_E = 30$. This figure corresponds to Fig. 6.

Figure 14 presents the simulation results for δ for scaling H_{SE} by the global interaction strength λ. From Fig. 14, it is obvious that we observe similar behavior for δ as we did for σ shown in Fig. 4 in the main text. The difference is in the stronger fluctuations for the data points for δ. There are two regimes of δ separated by some threshold number of N_E, labeled as $L(\lambda)$. If $N_E < L(\lambda)$, δ decreases approximately exponentially as N_E increases. If $N_E > L(\lambda)$, δ converges to a finite value that depends on λ. The constant values for δ for $N_E > L(\lambda)$ are well fitted to λ^2 (see the inset of Fig. 14). Figure 15 shows the simulation results for the fitting temperature b [see Eq. (7)] minus the inverse temperature β, where β is the inverse temperature used to prepare the canonical-thermal state of Eq. (11) from the initial state X. The data points fit well to $-\lambda^2$ for $\lambda < 1$. This implies that only for $\lambda \to 0$ (the uncoupled entirety) does one have $b = \beta$, which is consistent with the analysis for σ in the main text.

Figure 16 presents the simulation results for δ by varying the inverse temperature β that is used in Eq. (11) to obtain the canonical-thermal state from the state X. Figure 16 corresponds to Fig. 5 in the main text. We observe similar behavior for δ as we did for σ in the main text, except that there are larger fluctuations for the data points for δ. The converged values of δ for $N_E = 36$ is better fit to $(\beta|J|)^{3.18}$, which is slightly different from the fitting index for the converged values of σ. However, a definitive analysis of how robust the difference is would require high statistics calculations with averages over different times, different H_E, and different samples of the X state. Figure 17 shows the simulation results of the fitting temperature b with β subtracted. The data points

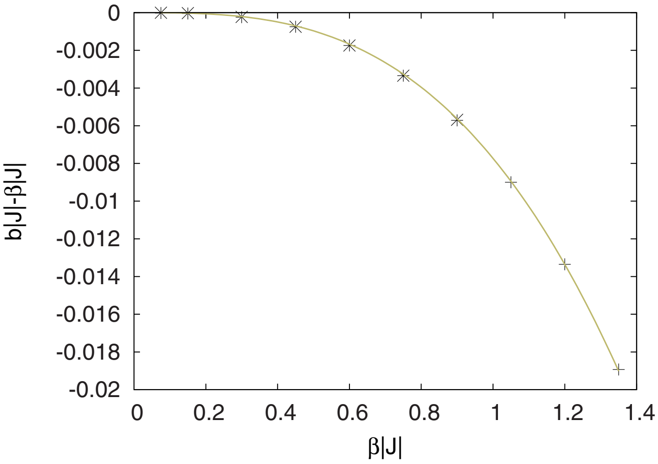

FIG. 17. Simulation results corresponding to Fig. 16 for the difference between the fitting temperature b and the inverse temperature β for entireties with $N_E = 26$ (pluses) and $N_E = 36$ (crosses). For $\beta|J| < 1$, the data points fit to $b|J| - \beta|J| \approx -0.007\,73\beta^3|J|^3$ (solid curve).

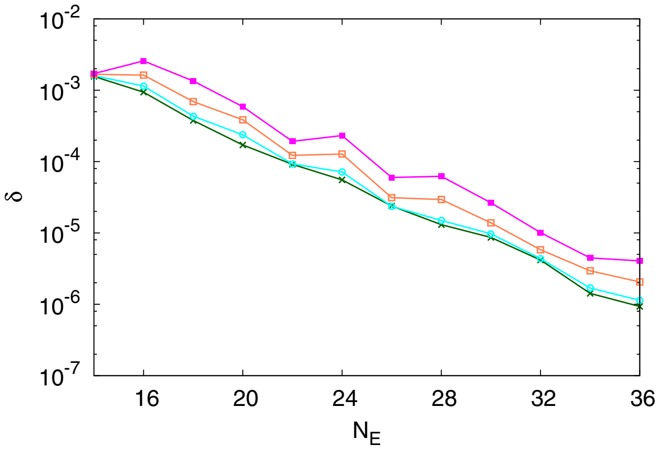

FIG. 19. Simulation results for δ for an uncoupled entirety ($\lambda = 0$), with $N_S = 4$ and $N_E = 14,\ldots,36$ for different inverse temperatures. Curves from bottom to top correspond to $\beta|J| = 0.075$, 0.30, 0.60, and 0.90. This figure corresponds to Fig. 7 in the main text.

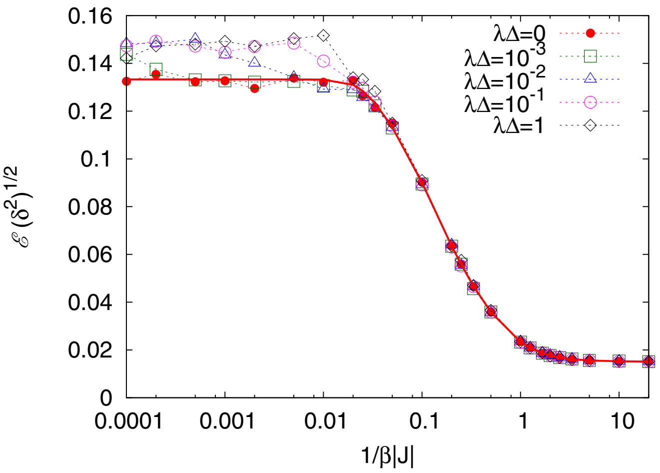

FIG. 20. Simulation results of $\sqrt{\mathscr{E}(\delta^2)}$ for ferromagnetic spin-$\frac{1}{2}$ chains with $N_S = 4$ and $N_E = 8$, $J = \Omega = 1$, and various interaction strengths $\lambda\Delta$ as a function of the temperature $T/J = 1/(\beta J)$. The solid line (red) is obtained from Eq. (29) by using numerical values for the free energies $F_S(n\beta)$ and $F_E(n\beta)$. The dotted lines are guides for the eye. Note that the functional form of the $\lambda = 0$ curve, as well as how data for finite λ relate to this curve, are very similar to Fig. 8 for σ.

for $\beta|J| < 1$ fit well to $-(\beta|J|)^3$, just as did the values in the main text for σ.

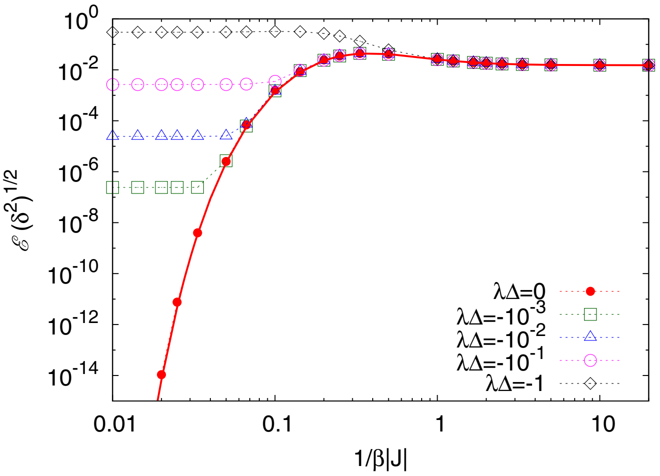

FIG. 21. Simulation results for $\sqrt{\mathscr{E}(\delta^2)}$ for spin-$\frac{1}{2}$ chains with $N_S = 4$, $N_E = 8$, $J = -1$, $\Omega = 1$, and various interaction strengths $\lambda\Delta$ as a function of temperature $T/|J| = 1/\beta|J|$. The solid line (red) is obtained from Eq. (29) by using numerical values for the free energies $F_S(n\beta)$ and $F_E(n\beta)$. The dotted lines are guides for the eye. Note that this figure is for $g_S = 1$, which looks very different compared to Fig. 20 for $g_S > 1$. This figure for δ corresponds to Fig. 9 for σ.

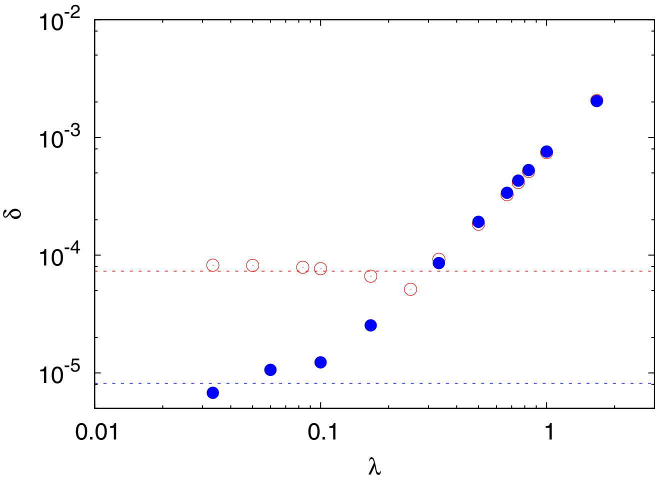

FIG. 22. Simulation results for δ for rings with $N_S = 4$, $N_E = 26$ (open circles) and $N_S = 4$, $N_E = 36$ (solid circles) as a function of the global interaction strength λ for $\beta|J| = 0.90$. The top (bottom) horizontal dashed line represents the value obtained by simulating the noninteraction system, $\lambda = 0$, with 30 (40) spins. This figure corresponds to Fig. 10 in the main text.

Figure 18 presents the corresponding results for δ to compare with results shown in Fig. 6 for σ. We see similar convergent behavior for both σ and δ when the environment size N_E is larger than a certain threshold value. For N_E smaller than the threshold value, δ decreases approximately exponentially with increasing N_E. Unlike the data points of σ which overlapped for this regime, the data points of δ do not overlap. This is because σ is only related to the factor from the environment [see Eqs. (8) and (27) in the main text], while δ is also related to the factor of the dimension of the Hilbert space from the system itself [see Eqs. (8) and (29) in the main text].

Figure 19 presents the corresponding results for δ, as shown in Fig. 7 for σ. It is clear that, except for strong fluctuations, δ for the uncoupled entirety ($\lambda = 0$) scales with the size of N_E.

Figures 20 and 21 present the simulation results for $\sqrt{\mathscr{E}(\delta^2)}$ obtained by exact diagonalization for the entirety $S + E$ being a spin chain with $N_S = 4$ and $N_E = 8$. These figures correspond to Figs. 8 and 9 in the main text. The data points are averaged over 1000 runs with different representations of the state X at specific temperature β. Therefore, the simulation results shown in Figs. 20 and 21 have very good statistics. We refer to the detailed discussion about these figures in the main text, as σ and δ behave very similarly. We remind the reader that both Figs. 20 and 8 are for the case with the ground-state degeneracy of the system being $g_S = 5$. We remind the reader that both Figs. 21 and 9 are for the case with the ground-state degeneracy of the system being $g_S = 1$. Figure 21 for $g_S = 1$ looks completely different from Fig. 20 for $g_S > 1$. Nevertheless, as the system-environment coupling strength $\lambda\Delta$ becomes small, the data from the calculations fall nicely on the theoretical curve obtained from Eq. (29) in the main text (red solid line). The theoretical curve for δ in the limit $T \to 0$, as seen in Eq. (39), is equal to zero. Note the extremely small values for $\sqrt{\mathscr{E}(\delta^2)}$ for low temperatures. Calculating the theoretical curves (red solid lines) for these quantities at low temperatures required quadruple precision in the floating point numbers.

Figure 22 presents the corresponding simulation results for δ as shown in Fig. 10 for σ. Note that there is no fitting procedure for these data points. The dashed lines, as in the main text, are for the uncoupled entirety, $\lambda = 0$. The behavior for δ here is quite similar to the behavior of σ in Fig. 10.

APPENDIX B: PERTURBATION THEORY

In this Appendix the details of the perturbation theory calculations are presented. Additional definitions and important considerations are first given.

1. Hamiltonian

The Hamiltonian has the form

$$H = H_S + H_E + \lambda H_{SE} = H_0 + \lambda H_I, \tag{B1}$$

where λ is explicitly written as the perturbation parameter and the uncoupled Hamiltonian is $H_0 = H_S + H_E$. The dimension of the Hilbert space of the environment, the system, and the entirety $S + E$ is D_E, D_S, and $D = D_S D_E$.

2. Random state

Any state from the Hilbert space of H can be written as the wave function

$$|\Psi_0\rangle = \sum_{k=1}^{D} d_k |E_k\rangle, \tag{B2}$$

where $\{|E_k\rangle\}$ form the energy basis of H. Random states in the Hilbert space of the entirety Hamiltonian H are obtained from Eq. (B2) if $\{d_k\}$ are random Gaussian coefficients, normalized to unity,

$$\sum_{k=1}^{D} d_k^* d_k \;=\; 1. \tag{B3}$$

In practice, in our computer program we generate the Gaussian random numbers $d_k = c_k + i b_k$ by using the Box-Muller method [61] to generate two Gaussian random numbers c_k' and b_k',

$$c_k' = \sqrt{-2\ln(r_0)}\cos(2\pi r_1) \quad \text{and} \quad b_k' = \sqrt{-2\ln(r_0)}\sin(2\pi r_1), \tag{B4}$$

where r_0 and r_1 are two independent random numbers distributed uniformly on $[0,1)$, so that the Gaussian random number d_k is given by simple normalization,

$$d_k \;=\; c_k + i b_k = \frac{c_k' + i b_k'}{\sqrt{\sum_{k'=1}^{D}[(c_{k'}')^2 + (b_{k'}')^2]}} = \sqrt{x_k} e^{i\phi_k}. \tag{B5}$$

The ensemble of random states has been previously analyzed [40] and has given predictions for measures of quantum decoherence and thermalization at infinite temperature ($\beta = 0$) [39].

3. Canonical-thermal state

One forms a wave function at finite inverse temperature β given by

$$|\Psi_\beta\rangle = \frac{e^{-\frac{\beta H}{2}}|\Psi_0\rangle}{\langle\Psi_0|e^{-\beta H}|\Psi_0\rangle^{1/2}}, \tag{B6}$$

which defines the ensemble of canonical-thermal states of Eq. (11). Here the inverse temperature is $\beta = 1/k_B T$ for temperature T, and we set Boltzmann's constant $k_B = 1$. Equation (B6) can be rewritten as

$$|\Psi_\beta\rangle = \frac{\sum_{k=1}^{D} d_k e^{-\frac{\beta E_k}{2}}|E_k\rangle}{\left[\sum_{k'=1}^{D} d_{k'}^* d_{k'} e^{-\beta E_{k'}}\right]^{\frac{1}{2}}} \tag{B7}$$

$$= \frac{d_1 e^{-\frac{\beta E_1}{2}}|E_1\rangle + \sum_{k=2}^{D} d_k e^{-\frac{\beta E_k}{2}}|E_k\rangle}{\left[d_1^* d_1 e^{-\beta E_1} + \sum_{k'=2}^{D} d_{k'}^* d_{k'} e^{-\beta E_{k'}}\right]^{\frac{1}{2}}} \tag{B8}$$

$$= \frac{d_1|E_1\rangle + \sum_{k=2}^{D} d_k e^{-\frac{\beta(E_k - E_1)}{2}}|E_k\rangle}{\left[d_1^* d_1 + \sum_{k'=2}^{D} d_{k'}^* d_{k'} e^{-\beta\left(E_{k'} - E_1\right)}\right]^{\frac{1}{2}}}, \tag{B9}$$

so that it becomes obvious that in the infinite-temperature ($\beta \to 0$) limit

$$\lim_{\beta\to 0}|\Psi_\beta\rangle = |\Psi_0\rangle. \tag{B10}$$

A canonical-thermal state is drawn from the distribution given by the canonical-thermal-state ensemble of Eq. (B6).

The canonical-thermal state can also be written as

$$|\Psi_\beta\rangle = \sum_{k=1}^{D} \frac{d_k e^{-\beta E_k/2}|E_k\rangle}{\sqrt{\sum_{k'=1}^{D}|d_{k'}|^2 e^{-\beta E_{k'}}}} = \sum_{k=1}^{D} a_k |E_k\rangle, \tag{B11}$$

with

$$a_k = \frac{d_k e^{-\beta E_k/2}}{\sqrt{\sum_{k'=1}^{D}|d_{k'}|^2 e^{-\beta E_{k'}}}} \tag{B12}$$

$$= \frac{d_k \; p_k^{1/2}}{\sqrt{\sum_{k'=1}^{D}|d_{k'}|^2 p_{k'}}}, \tag{B13}$$

with the Boltzmann probability of being in state k given by

$$p_k = \frac{e^{-\beta E_k}}{\sum_{k'=1}^{D} e^{-\beta E_{k'}}} = \frac{e^{-\beta E_k}}{Z}. \tag{B14}$$

The partition function of the entirety $S + E$ is given by

$$Z = \mathrm{Tr}_{S+E}(e^{-\beta H}) = \sum_{k=1}^{D} e^{-\beta E_k}. \tag{B15}$$

4. Canonical-thermal state for uncoupled entirety

For the uncoupled case, $\lambda = 0$, one has

$$|\Psi_\beta\rangle = \frac{d_{1,1}\big|E_1^{(S)}\big\rangle\big|E_1^{(E)}\big\rangle + \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} d_{i,p}(1 - \delta_{i,1}\delta_{p,1}) e^{-\frac{\beta(E_i^{(S)} - E_1^{(S)})}{2}} e^{-\frac{\beta(E_p^{(E)} - E_1^{(E)})}{2}}\big|E_i^{(S)}\big\rangle\big|E_p^{(E)}\big\rangle}{\left[d_{1,1}^* d_{1,1} + \sum_{i'=1}^{D_S}\sum_{p'=1}^{D_E} d_{i',p'}^* d_{i',p'}(1 - \delta_{i',1}\delta_{p',1}) e^{-\beta(E_{i'}^{(S)} - E_1^{(S)})} e^{-\beta(E_{p'}^{(E)} - E_1^{(E)})}\right]^{\frac{1}{2}}}, \tag{B16}$$

where $\{|E_i^{(S)}\rangle\}$ and $\{|E_p^{(E)}\rangle\}$ form the energy basis of H_S and H_E, respectively.

The canonical-thermal state for the uncoupled entirety can also be written as

$$|\Psi_\beta\rangle = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} \frac{d_{i,p}\, e^{-\beta E_i^{(S)}/2}\, e^{-\beta E_p^{(E)}/2}\, \big|E_i^{(S)}\big\rangle\big|E_p^{(E)}\big\rangle}{\sqrt{\sum_{i'=1}^{D_S}\sum_{p'=1}^{D_E} |d_{i',p'}|^2 e^{-\beta E_{i'}^{(S)}}\, e^{-\beta E_{p'}^{(E)}}}} = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} a_{i,p}\big|E_i^{(S)}\big\rangle\big|E_i^{(E)}\big\rangle, \tag{B17}$$

with

$$a_{i,p} = \frac{d_{i,p}\, e^{-\beta E_i^{(S)}/2}\, e^{-\beta E_p^{(E)}/2}}{\sqrt{\sum_{i'=1}^{D_S}\sum_{p'=1}^{D_E} |d_{i',p'}|^2 e^{-\beta E_{i'}^{(S)}}\, e^{-\beta E_{p'}^{(E)}}}} \tag{B18}$$

$$= \frac{d_{i,p}\sqrt{p_i^{(S)}}\sqrt{p_p^{(E)}}}{\sqrt{\sum_{i'=1}^{D_S}\sum_{p'=1}^{D_E} \big|d_{i',p'}\big|^2 p_{i'}^{(S)} p_{p'}^{(E)}}}, \tag{B19}$$

where the Boltzmann probability of being in state i of H_S is given by

$$p_i^{(S)} = \frac{e^{-\beta E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}} = \frac{e^{-\beta E_i^{(S)}}}{Z_S} \tag{B20}$$

and the Boltzmann probability of being in state p of H_E is given by

$$p_p^{(E)} = \frac{e^{-\beta E_p^{(E)}}}{\sum_{p'=1}^{D_E} e^{-\beta E_{p'}^{(E)}}} = \frac{e^{-\beta E_p^{(E)}}}{Z_E}. \tag{B21}$$

The partition function of the system is given by

$$Z_S(\beta) = \mathrm{Tr}_S(e^{-\beta H_S}) = \sum_{i=1}^{D_S} e^{-\beta E_i^{(S)}} \tag{B22}$$

and the partition function of the environment is given by

$$Z_E(\beta) = \mathrm{Tr}_E(e^{-\beta H_E}) = \sum_{p=1}^{D_E} e^{-\beta E_p^{(E)}}. \tag{B23}$$

Important to note is that, even though for the uncoupled case ($\lambda = 0$) the Hamiltonians H_S and H_E are uncoupled, the state of the entirety $S + E$ in Eq. (B17) is entangled since $d_{i,p} \neq d_i d_p$ for the random Gaussian variables. As described in the main text, there are ways to achieve this condition physically, for example, by using a much larger quantum bath that couples simultaneously to S and E and then slowly removing this large quantum bath.

5. Reduced density matrix

The density matrix for the entirety $S + E$ is ρ. The reduced density matrix $\widetilde{\rho}$ for S, written in the basis $\{|E_i^{(S)}\rangle\}$ that diagonalizes H_S, is defined by a partial trace over the environment, and has matrix elements (for any λH_{SE}) given by

$$\big\langle E_i^{(S)}\big|\widetilde{\rho}\big|E_{i'}^{(S)}\big\rangle = \widetilde{\rho}_{i,i'} = \big\langle E_i^{(S)}\big|\mathrm{Tr}_E(\rho)\big|E_{i'}^{(S)}\big\rangle = \sum_{p=1}^{D_E}\big\langle E_i^{(S)}\big|(\langle p|\rho|p\rangle)\big|E_{i'}^{(S)}\big\rangle \tag{B24}$$

for any complete orthonormal basis $\{|p\rangle\}$ that spans the Hilbert space of the environment. The reduced density matrix elements $\widetilde{\rho}_{i,i'}$ in the energy basis that diagonalizes H_S are thus

$$\widetilde{\rho}_{i,i'} = \sum_{p=1}^{D_E} \frac{\Big[d_{1,1}^*\delta_{i,1}\delta_{p,1} + d_{i,p}^*(1-\delta_{i,1}\delta_{p,1})e^{-\frac{\beta(E_i^{(S)}-E_1^{(S)})}{2}}e^{-\frac{\beta(E_p^{(E)}-E_1^{(E)})}{2}}\Big]\Big[d_{1,1}\delta_{i',1}\delta_{p,1} + d_{i',p}(1-\delta_{i',1}\delta_{p,1})e^{-\frac{\beta(E_{i'}^{(S)}-E_1^{(S)})}{2}}e^{-\frac{\beta(E_p^{(E)}-E_1^{(E)})}{2}}\Big]}{d_{1,1}^* d_{1,1} + \sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E} d_{i'',p''}^* d_{i'',p''}(1-\delta_{i'',1}\delta_{p'',1})e^{-\beta(E_{i''}^{(S)}-E_1^{(S)})}e^{-\beta(E_{p''}^{(E)}-E_1^{(E)})}}. \tag{B25}$$

Equation (B25) can be rewritten as

$$\widetilde{\rho}_{i,i'} = \sum_{p=1}^{D_E} \frac{d_{i,p}^* d_{i',p} e^{-\beta E_i^{(S)}/2} e^{-\beta E_{i'}^{(S)}/2} e^{-\beta E_p^{(E)}}}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E} d_{i'',p''}^* d_{i'',p''} e^{-\beta E_{i''}^{(S)}}\, e^{-\beta E_{p''}^{(E)}}}. \tag{B26}$$

Care must be taken that for $d_{i,p}$, $d_{i',p}$, and $d_{i'',p''}$ the value of the random variable is the same wherever the indices are the same. For example, the random number $d_{2,10}$ should be the same in both the numerator and the denominator.

6. Expressions for the random Gaussian variables

For the random Gaussian variables d_k, as defined in Eq. (B5), the ϕ_k for different k are independent random variables distributed uniformly in $[0,2\pi)$. Furthermore, the probability density function (pdf) is given by

$$\mathrm{pdf}(\phi) = \frac{1}{2\pi} \tag{B27}$$

so that the expectation values for the ϕ_k read

$$\begin{aligned}
\mathscr{E}(e^{i\phi}) &= \int_0^{2\pi} e^{i\phi}\mathrm{pdf}(\phi)d\phi \\
&= \frac{1}{2\pi}\int_0^{2\pi}[\cos(\phi)+i\,\sin(\phi)]d\phi = 0, \\
\mathscr{E}(e^{im\phi}) &= \int_0^{2\pi} e^{im\phi}\mathrm{pdf}(\phi)d\phi \\
&= \frac{1}{2\pi}\int_0^{2\pi}[\cos(m\phi)+i\,\sin(m\phi)]d\phi = 0, \\
\mathscr{E}(e^{i\phi_k}e^{+i\phi_{k'}}) &= \mathscr{E}(e^{i\phi_k})\mathscr{E}(e^{+i\phi_{k'}}) = 0 \quad \text{for } k \neq k', \\
\mathscr{E}(e^{i\phi_k}e^{-i\phi_{k'}}) &= \mathscr{E}(e^{i\phi_k})\mathscr{E}(e^{-i\phi_{k'}}) = 0 \quad \text{for } k \neq k', \\
\mathscr{E}(e^{i\phi_k}e^{-i\phi_{k'}}) &= \mathscr{E}(1) = 1 \qquad\qquad\qquad \text{for } k = k',
\end{aligned} \tag{B28}$$

which greatly simplifies the perturbation calculations performed in this section. Note that all expectation values for d_k are zero unless they are expectation values only for the absolute value $|d_k|^2 = d_k^* d_k = x_k$ of the Gaussian random variables.

For independent Gaussian random numbers (not our case, as we discuss below in this section), the distribution of the $|d|^2$ is given by a complete error function, defined by

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty e^{-t^2}dt. \tag{B29}$$

One can show this by using inverse transform sampling. In particular, the distribution for any $|d_1|^2$ is assumed to be, with the definition $x_1 = |d_1|^2$,

$$\mathrm{pdf}(x_1) = \frac{\pi D}{4}\mathrm{erfc}\left(\frac{D\sqrt{\pi}}{4}x_1\right). \tag{B30}$$

For independent $\{x_k\}$, the expectation values are

$$\begin{aligned}
\mathscr{E}(x) &= \int_0^\infty x\mathrm{pdf}(x)dx \\
&= \frac{\pi D}{4}\int_0^\infty x\ \mathrm{erfc}\left(\frac{D\sqrt{\pi}}{4}dx\right)dx = \frac{1}{D}, \\
\mathscr{E}(x^2) &= \int_0^\infty x^2\mathrm{pdf}(x)dx \\
&= \frac{\pi D}{4}\int_0^\infty x^2\mathrm{erfc}\left(\frac{D\sqrt{\pi}}{4}dx\right)dx = \frac{16}{3\pi D^2}, \\
\mathscr{E}(x_i x_j) &= \mathscr{E}(x_i)\mathscr{E}(x_j) = \frac{1}{D^2}, \\
\mathscr{E}(x^3) &= \int_0^\infty x^3\mathrm{pdf}(x)dx \\
&= \frac{\pi D}{4}\int_0^\infty x^3\mathrm{erfc}\left(\frac{D\sqrt{\pi}}{4}dx\right)dx = \frac{12}{\pi D^3}, \\
\mathscr{E}(x^4) &= \int_0^\infty x^4\mathrm{pdf}(x)dx \\
&= \frac{\pi D}{4}\int_0^\infty x^4\mathrm{erfc}\left(\frac{D\sqrt{\pi}}{4}dx\right)dx = \frac{512}{5\pi^2 D^4}.
\end{aligned} \tag{B31}$$

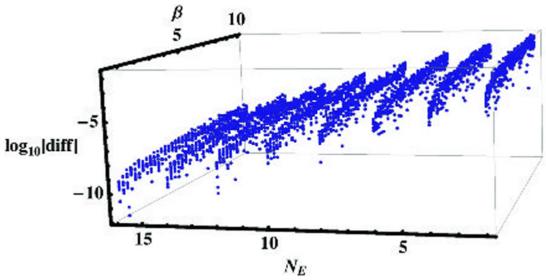

FIG. 23. Examples illustrating the approximation in Eq. (B34). The system is taken to have a Hilbert space of dimension $D_S = 2^4$. The environment is taken to have a Hilbert space of dimension $D_S = 2^{N_E}$, for $N_E = 2,4,6,8,10,12,14,16$. The values of β shown are from $\beta = 0.25$ to $\beta = 10$ in steps of 0.25. Here diff $= |(\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}|d_{i,p}|^2 p_i^{(S)} p_p^{(E)}) - \frac{1}{D}|$. The eigenvalues for both E and S were taken to be random numbers uniformly distributed in $[-2,1]$. There are 10 points at each value of N_E and β, each with different random eigenvalues for both S and E, as well as different Gaussian random numbers $d_{i,p}$.

The expressions in Eq. (B31) are only approximately correct for our case. The reason is that the pdf for D components of the random variables is given by

$$\frac{1}{\text{normalization}}\mathrm{pdf}(x_1)\mathrm{pdf}(x_2)\cdots \mathrm{pdf}(x_D)\delta(x_1+x_2+\cdots+x_D-1), \tag{B32}$$

where the normalization is complicated. However, Hams and De Raedt [40] have calculated the correct expectation values for the pdf in Eq. (B32), namely,

$$\mathscr{E}(x) = \frac{1}{D}, \quad \mathscr{E}(x^2) = \frac{2}{D(D+1)}, \quad \mathscr{E}(x_i x_j) = \frac{1}{D(D+1)}. \tag{B33}$$

Therefore, we do not have to calculate these expectation values, but rather just use these results from [40].

For sufficiently large D we can use the approximation (see Fig. 23)

$$\sum_{k=1}^{D}|d_k|^2 p_k \approx \frac{1}{D}, \tag{B34}$$

or by changing indices for the uncoupled case,

$$\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}|d_{i,p}|^2 p_{i,p} = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E}|d_{i,p}|^2 p_i^{(S)} p_p^{(E)} \approx \frac{1}{D}. \tag{B35}$$

Note that Eq. (B34) becomes exact in the infinite-temperature limit ($\beta \to 0$), where $p_k = 1/D$ for all k so

$$\lim_{\beta\to 0}\sum_{k=1}^{D}|d_k|^2 p_k = \frac{1}{D}\sum_{k=1}^{D}|d_k|^2 = \frac{1}{D}. \tag{B36}$$

In the zero-temperature limit ($\beta \to +\infty$) Eq. (B34) also becomes exact. Let g_1 be the ground-state degeneracy of the entirety Hamiltonian H associated with energy E_1. Then

$$\lim_{\beta\to\infty} p_k = \lim_{\beta\to\infty} \frac{e^{-\beta E_k}}{Z} = \lim_{\beta\to\infty} \frac{e^{-\beta E_k}}{g_1 e^{-\beta E_1} + \sum_{k'=1+g_1}^{D} e^{-\beta E_{k'}}}$$

$$= \begin{cases} \frac{1}{g_1} & k = 1,2,\ldots,g_1, \\ 0 & k = g_1+1, g_1+2, \ldots, D. \end{cases} \tag{B37}$$

Hence, the expectation value is

$$\lim_{\beta\to\infty} \mathscr{E}\left(\sum_{k=1}^{D} |d_k|^2 p_k\right) = \lim_{\beta\to\infty} \sum_{k=1}^{D} \mathscr{E}(|d_k|^2) p_k = \frac{1}{g_1}\sum_{k=1}^{g_1} \mathscr{E}(|d_k|^2)$$

$$= \frac{1}{g_1} g_1 \frac{1}{D} = \frac{1}{D}. \tag{B38}$$

The approximation given by Eq. (B34) is an uncontrolled approximation, and therefore we do not use it in our derivation of the perturbation theory for either σ or δ. We have included the results here because the approximation was discussed in the main text as a way to motivate our perturbation results obtained without using the approximation.

7. General procedure for Taylor expansion: General function

We need to calculate expectation values for the x_i for a general function. We can do a Taylor expansion about $x_i = 1/D$ and take the expectation value with respect to the probability distribution of the x_i or d_i denoted by $\mathscr{E}(\cdot)$:

$$\begin{aligned}
\mathscr{E}(f(\{x\})) = {} & f\left(\frac{1}{D},\frac{1}{D},\ldots,\frac{1}{D}\right) \\
& + \sum_{\ell=1}^{D} \frac{\partial f(x_1,x_2,\ldots,x_D)}{\partial x_\ell}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\right) \\
& + \frac{1}{2!}\sum_{\ell=1}^{D} \frac{\partial^2 f(x_1,x_2,\ldots,x_D)}{\partial x_\ell^2}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)^2\right) \\
& + \frac{1}{2!}\sum_{\ell=1}^{D}\sum_{\ell'=1}^{D} (1-\delta_{\ell,\ell'}) \frac{\partial^2 f(x_1,x_2,\ldots,x_D)}{\partial x_\ell \partial x_{\ell'}}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\left(x_{\ell'} - \frac{1}{D}\right)\right) \\
& + \frac{1}{3!}\sum_{\ell=1}^{D} \frac{\partial^3 f(x_1,x_2,\ldots,x_D)}{\partial x_\ell^3}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)^3\right) \\
& + \frac{1}{3!}\sum_{\ell=1}^{D}\sum_{\ell'=1}^{D}\sum_{\ell''=1}^{D} (\delta_{\ell,\ell'} + \delta_{\ell,\ell''} + \delta_{\ell',\ell''})(1 - \delta_{\ell,\ell'}\delta_{\ell,\ell''}\delta_{\ell',\ell''}) \\
& \times \frac{\partial^3 f(x_1,x_2,\ldots,x_D)}{\partial x_\ell \partial x_{\ell'} \partial x_{\ell''}}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\left(x'_\ell - \frac{1}{D}\right)\left(x''_\ell - \frac{1}{D}\right)\right) \\
& + \frac{1}{3!}\sum_{\ell=1}^{D}\sum_{\ell'=1}^{D}\sum_{\ell''=1}^{D} (1-\delta_{\ell,\ell'})(1-\delta_{\ell,\ell''})(1-\delta_{\ell',\ell''}) \\
& \times \frac{\partial^3 f(x_1,x_2,\ldots,x_D)}{\partial x_\ell \partial x_{\ell'} \partial x_{\ell''}}\bigg|_{\{x\}=\frac{1}{D}} \mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\left(x'_\ell - \frac{1}{D}\right)\left(x''_\ell - \frac{1}{D}\right)\right) \\
& + \text{higher-order terms.}
\end{aligned} \tag{B39}$$

Note that since the expectation values for quantities such as $\mathscr{E}(x_\ell^2)$ and $\mathscr{E}(x_\ell x_{\ell'})$ are different, we had to write the second-order term as two terms: one for the same-ℓ's terms and one for the different-ℓ,ℓ' terms. For the same reason, the third-order term is written as three different terms, one with all-same ℓ's, one with all different ℓ's, and one with two and only two same-ℓ's. Then use the fact that the expectation values are known [40] using Eq. (B33), for example, up to second order,

$$
\begin{aligned}
\mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\right) &= 0, \\
\mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)^2\right) &= \mathscr{E}\left(x_\ell^2\right) - \frac{2}{D}\mathscr{E}(x_\ell) + \frac{1}{D^2} = \frac{D-1}{D^2(D+1)}, \\
\mathscr{E}\left(\left(x_\ell - \frac{1}{D}\right)\left(x_{\ell'} - \frac{1}{D}\right)\right) &= \mathscr{E}(x_\ell x_{\ell'}) - \frac{1}{D}\mathscr{E}(x_\ell) - \frac{1}{D}\mathscr{E}(x_{\ell'}) + \frac{1}{D^2} = -\frac{1}{D^2(D+1)} \quad \ell \neq \ell',
\end{aligned}
\tag{B40}
$$

and the derivatives of f can be calculated, at least via *Mathematica*.

8. Derivation of $\mathscr{E}(\delta^2)$ for the uncoupled entirety

We first derive the expectation value for $\mathscr{E}(\delta^2)$ since this is easier than the corresponding expectation value for σ. The ease is because only diagonal elements of $\widetilde{\rho}$ enter into the expression for δ, since we have the definition

$$
\delta^2 = \sum_{i=1}^{D_S}\left(\widetilde{\rho}_{i,i} - \frac{e^{-bE_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-bE_{i'}^{(S)}}}\right)^2, \tag{B41}
$$

with the fitting parameter b given by

$$
b = \frac{\sum_{i<j,E_i^{(S)}\neq E_j^{(S)}} \frac{\ln(\widetilde{\rho}_{i,i})-\ln(\widetilde{\rho}_{j,j})}{E_j^{(S)}-E_i^{(S)}}}{\sum_{i'<j',E_{i'}^{(S)}\neq E_{j'}^{(S)}} 1}. \tag{B42}
$$

Therefore, for δ^2 there are no ϕ_k terms in the Gaussian random numbers in Eq. (B5). This is because only the diagonal elements of the reduced density matrix given by

$$
\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) = \sum_{p=1}^{D_E} \frac{x_{i,p}\,p_{i,p}}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E} x_{i'',p''}\,p_{i'',p''}} \tag{B43}
$$

enter expressions for δ (while expressions for σ involve the off-diagonal elements of $\widetilde{\rho}_{i,j}$). Remember, care must be taken that, for both $x_{i,p}$ and $x_{i'',p''}$, wherever the indices are the same the value of the variable is the same. For example the random number $x_{1,1}$ is the same in both the numerator and the denominator.

Introduce $\Delta b = b - \beta$ with b the fitting parameter, so $b = \beta + \Delta b$.

The function we need to analyze is

$$
f_{\delta^2}(\beta,\Delta b,\{x_{i,p}\}) = \sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^S(\beta,\Delta b)\right]^2, \tag{B44}
$$

with the definition

$$
p_i^{(S)}(\beta,\kappa) = \frac{e^{(\beta+\kappa)E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{(\beta+\kappa)E_{i'}^{(S)}}}. \tag{B45}
$$

For the noninteracting case, $\lambda = 0$, we need to analyze the function Eq. (B44) with

$$
\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) = \sum_{p=1}^{D_E} \frac{x_{i,p}\,p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E} x_{i'',p''}\,p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)}. \tag{B46}
$$

For the lowest-order (zeroth-order) term in the Taylor expansion we replace all $x_{i,p}$ with $1/D$. This gives

$$
\begin{aligned}
\widetilde{\rho}_{i,i}\left(\beta,\{x_{i,p}\} = \frac{1}{D}\right) &= \sum_{p=1}^{D_E} \frac{\frac{1}{D}p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}\frac{1}{D}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)} = \sum_{p=1}^{D_E} \frac{p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E} p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)} \\
&= p_i^{(S)}(\beta,0)\sum_{p=1}^{D_E} p_p^{(E)}(\beta) = p_i^{(S)}(\beta,0),
\end{aligned}
\tag{B47}
$$

since $\sum_{i=1}^{D_S} p_i^{(S)}(\beta,0) = 1$ and $\sum_{p=1}^{D_E} p_p^{(E)}(\beta) = 1$. Thus, one has

$$f_{\delta^2}\left(\beta,\Delta b,\{x_{i,p}\} = \frac{1}{D}\right) = \sum_{i=1}^{D_S} \left[p_i^{(S)}(\beta,0) - p_i^{(S)}(\beta,\Delta b)\right]^2, \tag{B48}$$

which obviously has its minimum at $\Delta b = 0$. Therefore, we perform a Taylor expansion also about $\Delta b = 0$, as well as an expansion in the $\{x_{i,p}\}$ about $\frac{1}{D}$.

For the first-order terms we make use of the chain rule. This gives

$$\frac{\partial f_{\delta^2}}{\partial \Delta b} = -2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\frac{\partial p_i^{(S)}(\beta,\Delta b)}{\partial \Delta b} \tag{B49}$$

and

$$\frac{\partial f_{\delta^2}}{\partial x_{j,q}} = 2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\frac{\partial \widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}. \tag{B50}$$

Note that

$$\left.\frac{\partial f_{\delta^2}}{\partial \Delta b}\right|_{\Delta b=0,\{x_{i,p}\}=\frac{1}{D}} = 0 \tag{B51}$$

and

$$\left.\frac{\partial f_{\delta^2}}{\partial x_{j,q}}\right|_{\Delta b=0,\{x_{i,p}\}=\frac{1}{D}} = 0. \tag{B52}$$

Hence, we need to go to the second-order terms.

For Δb, this is

$$\frac{\partial^2 f_{\delta^2}}{\partial(\Delta b)^2} = 2\sum_{i=1}^{D_S}\left[\frac{\partial p_i^{(S)}(\beta,\Delta b)}{\partial \Delta b}\right]^2 - 2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\frac{\partial^2 p_i^{(S)}(\beta,\Delta b)}{\partial(\Delta b)^2}. \tag{B53}$$

Evaluating at $\Delta b = 0$ gives

$$\left.\frac{\partial^2 f_{\delta^2}}{\partial(\Delta b)^2}\right|_{\Delta b=0,\{x_{i,p}\}=\frac{1}{D}} = 2\sum_{i=1}^{D_S}\left.\left[\frac{\partial p_i^{(S)}(\beta,\Delta b)}{\partial \Delta b}\right]^2\right|_{\Delta b=0,\{x_{i,p}\}=\frac{1}{D}}. \tag{B54}$$

One has

$$\sum_{i=1}^{D_S}\left.\frac{\partial p_i^{(S)}(\beta,\Delta b)}{\partial \Delta b}\right|_{\Delta b=0} = \left.\frac{\partial}{\partial \Delta b}\left(\sum_{i=1}^{D_S}\frac{e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}}\right)\right|_{\Delta b=0} = \frac{\partial}{\partial \Delta b}(1)|_{\Delta b=0} = 0. \tag{B55}$$

However, the term one needs to sum for the second-order term of Eq. (B53) is

$$\begin{aligned}
2\sum_{i=1}^{D_S}\left.\left[\frac{\partial p_i^{(S)}(\beta,\Delta b)}{\partial \Delta b}\right]^2\right|_{\Delta b=0} &= 2\sum_{i=1}^{D_S}\left.\left[\frac{\partial}{\partial \Delta b}\frac{e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}}\right]^2\right|_{\Delta b=0}\\
&= 2\sum_{i=1}^{D_S}\left.\left[\frac{e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)}e^{-\beta E_{i''}^{(S)}}e^{-\Delta b E_{i''}^{(S)}}\right)}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}\right)^2} - \frac{E_i^{(S)}e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}\right)}\right]^2\right|_{\Delta b=0}\\
&= 2\sum_{i=1}^{D_S}\left.\left[\frac{e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)}e^{-\beta E_{i''}^{(S)}}e^{-\Delta b E_{i''}^{(S)}}\right)}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}\right)^2}\right]^2\right|_{\Delta b=0}\\
&\quad -4\sum_{i=1}^{D_S}\left.\left[\frac{e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)}e^{-\beta E_{i''}^{(S)}}e^{-\Delta b E_{i''}^{(S)}}\right)}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}\right)^2}\frac{E_i^{(S)}e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}\right)}\right]\right|_{\Delta b=0}\\
&\quad +2\sum_{i=1}^{D_S}\left.\left[\frac{E_i^{(S)}e^{-\beta E_i^{(S)}}e^{-\Delta b E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}e^{-\Delta b E_{i'}^{(S)}}}\right]^2\right|_{\Delta b=0}
\end{aligned}$$

$$\begin{aligned}
&= 2\sum_{i=1}^{D_S}\left[\frac{e^{-\beta E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)} e^{-\beta E_{i''}^{(S)}}\right)}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}\right)^2}\right]^2 \\
&\quad - 4\sum_{i=1}^{D_S}\left[\frac{e^{-\beta E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)} e^{-\beta E_{i''}^{(S)}}\right)}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}\right)^2}\frac{E_i^{(S)} e^{-\beta E_i^{(S)}}}{\left(\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}\right)}\right] + 2\sum_{i=1}^{D_S}\left[\frac{E_i^{(S)} e^{-\beta E_i^{(S)}}}{\sum_{i'=1}^{D_S} e^{-\beta E_{i'}^{(S)}}}\right]^2 \\
&= 2\frac{1}{Z_S^4(\beta)}\sum_{i=1}^{D_S}\left[e^{-\beta E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)} e^{-\beta E_{i''}^{(S)}}\right)\right]^2 \\
&\quad - 4\frac{1}{Z_S^3(\beta)}\sum_{i=1}^{D_S}\left[e^{-\beta E_i^{(S)}}\left(\sum_{i''=1}^{D_S} E_{i''}^{(S)} e^{-\beta E_{i''}^{(S)}}\right)E_i^{(S)} e^{-\beta E_i^{(S)}}\right] + 2\frac{1}{Z_S^2(\beta)}\sum_{i=1}^{D_S}\left[E_i^{(S)} e^{-\beta E_i^{(S)}}\right]^2 \\
&= 2\frac{[\langle E(\beta)\rangle_S]^2 Z_S(2\beta)}{Z_S^2(\beta)} - 4\frac{\langle E(\beta)\rangle_S\langle E(2\beta)\rangle_S Z_S(2\beta)}{Z_S^2(\beta)} + 2\frac{\langle E^2(2\beta)\rangle_S Z_S(2\beta)}{Z_S^2(\beta)}.
\end{aligned} \tag{B56}$$

Therefore, the result for the first nonzero term for Δb is

$$\frac{1}{2!}\frac{\partial^2 f_{\delta^2}}{\partial(\Delta b)^2}\bigg|_{\Delta b=0,\{x_{i,p}\}=\frac{1}{D}}(\Delta b)^2 = \frac{Z_S(2\beta)}{Z_S^2(\beta)}\{[\langle E(\beta)\rangle_S]^2 - 2\langle E(\beta)\rangle_S\langle E(2\beta)\rangle_S + \langle E^2(2\beta)\rangle_S\}(\Delta b)^2 + \text{higher-order terms.} \tag{B57}$$

Initially, one would anticipate that one needs to calculate terms such as

$$\frac{\partial^2 f_{\delta^2}}{\partial(\Delta b)\partial x_{j,q}} \tag{B58}$$

and evaluate them at $\Delta b = 0,\{x_{i,p}\} = \frac{1}{D}$. However, all such terms will be multiplied by $(x_{j,q} - \frac{1}{D})$, which has an expectation value which vanishes. Therefore, one has

$$\begin{aligned}
\mathscr{E}(\delta^2) = {}& \frac{Z_S(2\beta)}{Z_S^2(\beta)}\{[\langle E(\beta)\rangle_S]^2 - 2\langle E(\beta)\rangle_S\langle E(2\beta)\rangle_S + \langle E^2(2\beta)\rangle_S\}(\Delta b)^2 + \mathscr{O}((\Delta b)^3) + \mathscr{O}((\Delta b)\{x_{j,q}\}^2) \\
& + \mathscr{O}(\{x_{j,q}\}\{x_{j',q'}\}(1-\delta_{j,j'}\delta_{q,q'})) + \mathscr{O}(\{x_{j,q}\}^2).
\end{aligned} \tag{B59}$$

One can also use that the specific heat (at constant volume) is $C_v(\beta) = k_B\beta^2\langle[\Delta E(\beta)]^2\rangle$, so

$$\langle E^2(2\beta)\rangle = \frac{C_v(2\beta)}{4k_B\beta^2} + [\langle E(2\beta)\rangle]^2. \tag{B60}$$

The final result is consequently

$$\begin{aligned}
\mathscr{E}(\delta^2) = {}& \frac{Z_S(2\beta)}{Z_S^2(\beta)}\left\{\frac{1}{4k_B\beta^2}C_v^{(S)}(2\beta) + [\langle E(2\beta)\rangle_S - \langle E(\beta)\rangle_S]^2\right\}(\Delta b)^2 + \mathscr{O}((\Delta b)^3) + \mathscr{O}((\Delta b)\{x_{j,q}\}^2) \\
& + \mathscr{O}(\{x_{j,q}\}\{x_{j',q'}\}(1-\delta_{j,j'}\delta_{q,q'})) + \mathscr{O}(\{x_{j,q}\}^2).
\end{aligned} \tag{B61}$$

Thus, equilibrating the system, in particular fitting for Δb, is difficult to do near a phase transition where C_v diverges.

For the second-order terms for the $\{x_{i,p}\}$ one has

$$\frac{\partial^2 f_{\delta^2}}{\partial x_{j,q}\partial x_{j',q'}} = 2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\frac{\partial^2\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}\partial x_{j',q'}} + 2\sum_{i=1}^{D_S}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j',q'}}. \tag{B62}$$

The derivative of $\widetilde{\rho}_{i,i}$ with respect to $\{x_{j,q}\}$ is given by

$$\begin{aligned}
\frac{\partial\widetilde{\rho}_{i,i}}{\partial x_{j,q}} &= \frac{\partial}{\partial x_{j,q}}\left[\sum_{p=1}^{D_E}\frac{x_{i,p}p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)}\right] \\
&= \delta_{i,j}\frac{p_i^{(S)}(\beta,0)p_q^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)} - \sum_{p=1}^{D_E}\frac{x_{i,p}p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)p_j^{(S)}(\beta,0)p_q^{(E)}(\beta)}{\left[\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)\right]^2}.
\end{aligned} \tag{B63}$$

Evaluating at $\{x_{i,p}\} = \frac{1}{D}$ gives

$$\begin{aligned}
\left.\frac{\partial \widetilde{\rho}_{i,i}}{\partial x_{j,q}}\right|_{\{x\}=\frac{1}{D}} &= \delta_{i,j}\frac{p_i^{(S)}(\beta,0)p_q^{(E)}(\beta)}{\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}\frac{1}{D}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)} - \sum_{p=1}^{D_E}\frac{\frac{1}{D}p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)p_j^{(S)}(\beta,0)p_q^{(E)}(\beta)}{\left[\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}\frac{1}{D}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)\right]^2}\\
&= D\delta_{i,j}p_i^{(S)}(\beta,0)p_q^{(E)}(\beta) - Dp_i^{(S)}(\beta,0)p_j^{(S)}(\beta,0)p_q^{(E)}(\beta)\sum_{p=1}^{D_E}p_p^{(E)}(\beta)\\
&= D\delta_{i,j}p_i^{(S)}(\beta,0)p_q^{(E)}(\beta) - Dp_i^{(S)}(\beta,0)p_j^{(S)}(\beta,0)p_q^{(E)}(\beta)\\
&= Dp_i^{(S)}(\beta,0)p_q^{(E)}(\beta)\left[\delta_{i,j} - p_j^{(S)}(\beta,0)\right],
\end{aligned} \tag{B64}$$

since $\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta) = 1$ and $\sum_{p=1}^{D_E}p_p^{(E)}(\beta) = 1$.

The second-order term for the same $x_{j,q}$ is

$$\begin{aligned}
\frac{\partial^2\widetilde{\rho}_{i,i}}{\partial x_{j,q}^2} = &-\delta_{i,j}\frac{\left[p_i^{(S)}(\beta,0)\right]^2\left[p_q^{(E)}(\beta)\right]^2}{\left[\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)\right]^2} - \delta_{i,j}\frac{\left[p_i^{(S)}(\beta,0)\right]^2\left[p_q^{(E)}(\beta)\right]^2}{\left[\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)\right]^2}\\
&+2\sum_{p=1}^{D_E}\frac{x_{i,p}p_i^{(S)}(\beta,0)p_p^{(E)}(\beta)\left[p_j^{(S)}(\beta,0)\right]^2\left[p_q^{(E)}(\beta)\right]^2}{\left[\sum_{i''=1}^{D_S}\sum_{p''=1}^{D_E}x_{i'',p''}p_{i''}^{(S)}(\beta,0)p_{p''}^{(E)}(\beta)\right]^3}.
\end{aligned} \tag{B65}$$

However, one does not need to calculate this term, since it only multiplies terms which are zero when $\Delta b = 0$ and $\{x_{i,p}\} = \frac{1}{D}$.

For the second-order term twice for the $\{x_{i,p}\}$ one has

$$\frac{\partial^2 f_{\delta^2}}{\partial(x_{j,q})^2} = 2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\frac{\partial^2\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial(x_{j,q})^2} + 2\sum_{i=1}^{D_S}\left[\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\right]^2. \tag{B66}$$

Hence,

$$\begin{aligned}
\left.\frac{\partial^2 f_{\delta^2}}{\partial(x_{j,q})^2}\right|_{\Delta b=0,\{x\}=\frac{1}{D}} &= 2\sum_{i=1}^{D_S}\left[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\}) - p_i^{(S)}(\beta,\Delta b)\right]\left.\frac{\partial^2\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial(x_{j,q})^2}\right|_{\Delta b=0,\{x\}=\frac{1}{D}} + 2\sum_{i=1}^{D_S}\left.\left[\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\right]^2\right|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&= 2\sum_{i=1}^{D_S}\left.\left[\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\right]^2\right|_{\Delta b=0,\{x\}=\frac{1}{D}} = 2\sum_{i=1}^{D_S}\left\{Dp_i^{(S)}(\beta,0)p_q^{(E)}(\beta)\left[\delta_{i,j} - p_j^{(S)}(\beta,0)\right]\right\}^2\\
&= 2D^2\left[p_q^{(E)}(\beta)\right]^2\sum_{i=1}^{D_S}\left[p_i^{(S)}(\beta,0)\right]^2\left[\delta_{i,j} - p_j^{(S)}(\beta,0)\right]^2\\
&= 2D^2\left[p_q^{(E)}(\beta)\right]^2\sum_{i=1}^{D_S}\left[p_i^{(S)}(\beta,0)\right]^2\left\{\delta_{i,j} - 2\delta_{i,j}p_j^{(S)}(\beta,0) + \left[p_j^{(S)}(\beta,0)\right]^2\right\}\\
&= 2D^2\left[p_q^{(E)}(\beta)\right]^2\left(\sum_{i=1}^{D_S}\delta_{i,j}\left[p_i^{(S)}(\beta,0)\right]^2 - 2\sum_{i=1}^{D_S}\delta_{i,j}\left[p_i^{(S)}(\beta,0)\right]^2p_j^{(S)}(\beta,0)\right.\\
&\qquad\left.+\left\{\left[p_j^{(S)}(\beta,0)\right]^2\sum_{i=1}^{D_S}\left[p_i^{(S)}(\beta,0)\right]^2\right\}\right)\\
&= 2D^2\left[p_q^{(E)}(\beta)\right]^2\left(\left[p_j^{(S)}(\beta,0)\right]^2 - 2\left[p_j^{(S)}(\beta,0)\right]^3 + \left[p_j^{(S)}(\beta,0)\right]^2\left\{\sum_{i=1}^{D_S}\left[p_i^{(S)}(\beta,0)\right]^2\right\}\right).
\end{aligned} \tag{B67}$$

We have to sum over all the same-second-partial terms to get the term that multiplies

$$\mathscr{E}\left(\left(x_{i,p} - \frac{1}{D}\right)^2\right) = \mathscr{E}\left(\left(x - \frac{1}{D}\right)^2\right) = \frac{D-1}{D^2(D+1)}, \tag{B68}$$

since these expectation values are the same for all $x_{i,p}$. One has

$$\begin{aligned}
&\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\frac{\partial^2 f_{\delta^2}}{\partial(x_{j,q})^2}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&= 2D^2\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\big[p_q^{(E)}(\beta)\big]^2\left(\big[p_j^{(S)}(\beta,0)\big]^2-2\big[p_j^{(S)}(\beta,0)\big]^3+\big[p_j^{(S)}(\beta,0)\big]^2\left\{\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\right\}\right)\\
&= 2D^2\left\{\sum_{q=1}^{D_E}\big[p_q^{(E)}(\beta)\big]^2\right\}\sum_{j=1}^{D_S}\left(\big[p_j^{(S)}(\beta,0)\big]^2-2\big[p_j^{(S)}(\beta,0)\big]^3+\big[p_j^{(S)}(\beta,0)\big]^2\left\{\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\right\}\right)\\
&= 2D^2\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\sum_{j=1}^{D_S}\left(\big[p_j^{(S)}(\beta,0)\big]^2-2\big[p_j^{(S)}(\beta,0)\big]^3+\big[p_j^{(S)}(\beta,0)\big]^2\left\{\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\right\}\right)\\
&= 2D^2\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left(\sum_{j=1}^{D_S}\big[p_j^{(S)}(\beta,0)\big]^2-2\sum_{j=1}^{D_S}\big[p_j^{(S)}(\beta,0)\big]^3+\left\{\sum_{j=1}^{D_S}\big[p_j^{(S)}(\beta,0)\big]^2\right\}\left\{\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\right\}\right)\\
&= 2D^2\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left(\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\left\{\sum_{j=1}^{D_S}\big[p_j^{(S)}(\beta,0)\big]^2\right\}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\right)\\
&= 2D^2\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right].
\end{aligned}\tag{B69}$$

Therefore, for these second-order terms the final result is that

$$\mathscr{E}\left(\left(x_{i,p}-\frac{1}{D}\right)^2\right)\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\frac{\partial^2 f_{\delta^2}}{\partial(x_{j,q})^2}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}} = 2\frac{D-1}{D+1}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right].\tag{B70}$$

For the second-order terms with two different $\{x_{i,p}\}$ one has

$$\frac{\partial^2 f_{\delta^2}}{\partial x_{j,q}\partial x_{j',q'}} = 2\sum_{i=1}^{D_S}\big[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})-p_i^{(S)}(\beta,\Delta b)\big]\frac{\partial^2\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}\partial x_{j',q'}}+2\sum_{i=1}^{D_S}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j',q'}}.\tag{B71}$$

Evaluating at $\Delta b=0$ and $\{x\}=\frac{1}{D}$ gives

$$\begin{aligned}
\frac{\partial^2 f_{\delta^2}}{\partial x_{j,q}\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}} &= 2\sum_{i=1}^{D_S}\big[\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})-p_i^{(S)}(\beta,\Delta b)\big]\frac{\partial^2\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&\quad+2\sum_{i=1}^{D_S}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&= 2\sum_{i=1}^{D_S}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j,q}}\frac{\partial\widetilde{\rho}_{i,i}(\beta,\{x_{i,p}\})}{\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&= 2\sum_{i=1}^{D_S}\big\{Dp_i^{(S)}(\beta,0)p_q^{(E)}(\beta)\big[\delta_{i,j}-p_j^{(S)}(\beta,0)\big]\big\}\big\{Dp_i^{(S)}(\beta,0)p_{q'}^{(E)}(\beta)\big[\delta_{i,j'}-p_{j'}^{(S)}(\beta,0)\big]\big\}\\
&= 2D^2\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\big[\delta_{i,j}-p_j^{(S)}(\beta,0)\big]\big[\delta_{i,j'}-p_{j'}^{(S)}(\beta,0)\big].
\end{aligned}\tag{B72}$$

We have to sum over all the different-$x_{i,p}$-second-partial terms to get the term that multiplies

$$\mathscr{E}\left(\left(x_{i,p}-\frac{1}{D}\right)\left(x_{i',p'}-\frac{1}{D}\right)\right)=\mathscr{E}\left(\left(x-\frac{1}{D}\right)\left(x'-\frac{1}{D}\right)\right)=-\frac{1}{D^2(D+1)},\tag{B73}$$

since these expectation values are the same for all pairs $x_{i,p}$ and $x_{i',p'}$. One has

$$
\begin{aligned}
&\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}(1-\delta_{j,j'}\delta_{q,q'})\frac{\partial^2 f_{\delta^2}}{\partial x_{j,q}\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&=2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}(1-\delta_{j,j'}\delta_{q,q'})\sum_{i=1}^{D_S}\big\{\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\big[\delta_{i,j}-p_j^{(S)}(\beta,0)\big]\big[\delta_{i,j'}-p_{j'}^{(S)}(\beta,0)\big]\big\}\\
&=2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}\sum_{i=1}^{D_S}\big\{\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\big[\delta_{i,j}-p_j^{(S)}(\beta,0)\big]\big[\delta_{i,j'}-p_{j'}^{(S)}(\beta,0)\big]\big\}\\
&\quad-2D^2\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\sum_{i=1}^{D_S}\big\{\big[p_i^{(S)}(\beta,0)\big]^2\big[p_q^{(E)}(\beta)\big]^2\big[\delta_{i,j}-p_j^{(S)}(\beta,0)\big]^2\big\}\\
&=2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\delta_{i,j}\delta_{i,j'}-2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\delta_{i,j}p_{j'}^{(S)}(\beta,0)\\
&\quad-2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)\delta_{i,j'}p_j^{(S)}(\beta,0)\\
&\quad+2D^2\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2 p_q^{(E)}(\beta)p_{q'}^{(E)}(\beta)p_j^{(S)}(\beta,0)p_{j'}^{(S)}(\beta,0)-2D^2\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\big[p_q^{(E)}(\beta)\big]^2\delta_{i,j}\\
&\quad+4D^2\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\big[p_q^{(E)}(\beta)\big]^2\delta_{i,j}p_j^{(S)}(\beta,0)-2D^2\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\big[p_q^{(E)}(\beta)\big]^2\big[p_j^{(S)}(\beta,0)\big]^2\\
&=2D^2\sum_{j,j'=1}^{D_S}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\delta_{i,j}\delta_{i,j'}-2D^2\sum_{j,j'=1}^{D_S}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\delta_{i,j}p_{j'}^{(S)}(\beta,0)\\
&\quad-2D^2\sum_{j,j'=1}^{D_S}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\delta_{i,j'}p_j^{(S)}(\beta,0)+2D^2\sum_{j,j'=1}^{D_S}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2 p_j^{(S)}(\beta,0)p_{j'}^{(S)}(\beta,0)\\
&\quad-2D^2\sum_{j=1}^{D_S}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\delta_{i,j}+4D^2\sum_{j=1}^{D_S}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\delta_{i,j}p_j^{(S)}(\beta,0)\\
&\quad-2D^2\sum_{j=1}^{D_S}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\big[p_j^{(S)}(\beta,0)\big]^2\\
&=2D^2\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2-2D^2\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2-2D^2\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\\
&\quad+2D^2\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2-2D^2\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2+4D^2\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^3\\
&\quad-2D^2\sum_{j=1}^{D_S}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\sum_{i=1}^{D_S}\big[p_i^{(S)}(\beta,0)\big]^2\big[p_j^{(S)}(\beta,0)\big]^2\\
&=-2D^2\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right],
\end{aligned}
\tag{B74}
$$

since $\sum_{q=1}^{D_E} p_q^{(E)}=1$ and $\sum_{j=1}^{D_S} p_j^{(S)}=1$.

Therefore, for these second-order terms the final result is that

$$\begin{aligned}
&\mathscr{E}\left(\left(x-\frac{1}{D}\right)\left(x'-\frac{1}{D}\right)\right)\sum_{j,j'=1}^{D_S}\sum_{q,q'=1}^{D_E}(1-\delta_{j,j'}\delta_{q,q'})\frac{\partial^2 f_{\delta^2}}{\partial x_{j,q}\partial x_{j',q'}}\bigg|_{\Delta b=0,\{x\}=\frac{1}{D}}\\
&=\left[-\frac{1}{D^2(D+1)}\right]\left\{-2D^2\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\\
&=\frac{2}{D+1}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right].
\end{aligned}\tag{B75}$$

Thus, the complete answer for $\mathscr{E}(\delta^2)$, to second order in Δb and all the $\{x\}$, is

$$\begin{aligned}
\mathscr{E}(\delta^2)&=\frac{1}{2!}\left\{2\frac{D-1}{D+1}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\\
&\quad+\frac{1}{2!}\left\{\frac{2}{D+1}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\\
&=\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\left[\frac{D-1}{D+1}+\frac{1}{D+1}\right]\\
&=\frac{D}{D+1}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right].
\end{aligned}\tag{B76}$$

In the infinite-temperature limit ($\beta=0$), one has that $Z_E(\beta\to 0)=D_E$ and $Z_S(\beta\to 0)=D_S$. Our expression then gives that

$$\lim_{\beta\to 0}\mathscr{E}(\delta^2)=\frac{D}{D+1}\frac{D_E}{D_E^2}\left(\frac{1}{D_S}-\frac{2}{D_S^2}+\frac{1}{D_S^2}\right)=\frac{D}{D+1}\frac{1}{D_E}\left(\frac{D_S-1}{D_S^2}\right)=\frac{D}{D+1}\frac{1}{D_E}\frac{1}{D_S}\left(\frac{D_S-1}{D_S}\right)=\frac{1}{D+1}\frac{D_S-1}{D_S},\tag{B77}$$

which is the same expression as we published in our 2013 paper [39], Eq. (C3).

One can also calculate how the low-temperature (high β) limit of $\mathscr{E}(\delta^2)$ is approached. However, one has to be cautious about the low-temperature ($\beta\to+\infty$) limit, since the analysis requires that $\beta\langle H_{SE}\rangle$ be small. Let g_S and g_E be the ground-state degeneracies of the Hamiltonians H_S and H_E associated with ground-state energies $E_1^{(S)}$ and $E_2^{(E)}$, respectively. Use that

$$\lim_{\beta\to\infty}\frac{Z_E(2\beta)}{Z_E^2(\beta)}=\lim_{\beta\to\infty}\frac{g_E e^{-2\beta E_1^{(E)}}+\sum_{p=1+g_E}^{D_E}e^{-2\beta E_p^{(E)}}}{\left(g_E e^{-\beta E_1^{(E)}}+\sum_{p'=1+g_E}^{D_E}e^{-\beta E_{p'}^{(E)}}\right)^2}=\lim_{\beta\to\infty}\frac{g_E+\sum_{p=1+g_E}^{D_E}e^{-2\beta(E_p^{(E)}-E_1^{(E)})}}{\left(g_E+\sum_{p'=1+g_E}^{D_E}e^{-\beta(E_{p'}^{(E)}-E_1^{(E)})}\right)^2}=\frac{g_E}{g_E^2}=\frac{1}{g_E}.\tag{B78}$$

Similarly, one has the limits

$$\lim_{\beta\to\infty}\frac{Z_S(2\beta)}{Z_S^2(\beta)}=\frac{1}{g_S},\quad\lim_{\beta\to\infty}\frac{Z_S(3\beta)}{Z_S^3(\beta)}=\frac{1}{g_S^2},\quad\lim_{\beta\to\infty}\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}=\frac{1}{g_S^2}.\tag{B79}$$

Hence, one has the low-temperature limit

$$\lim_{\beta\to\infty}\mathscr{E}(\delta^2)=\frac{1}{g_E}\frac{D}{D+1}\left(\frac{1}{g_S}-\frac{2}{g_S^2}+\frac{1}{g_S^2}\right)=\frac{1}{g_Sg_E}\frac{D}{D+1}\left(1-\frac{1}{g_S}\right)=\frac{g_S-1}{g_S^2g_E}\frac{D}{D+1}=\frac{g_S-1}{g_S^2g_E}\frac{1}{1+\frac{1}{D}}.\tag{B80}$$

In the limit of large D this becomes

$$\lim_{\beta\to\infty}\mathscr{E}(\delta^2)\approx\frac{g_S-1}{g_S^2g_E}.\tag{B81}$$

Therefore, in the low-temperature limit the expectation value goes to zero for $g_S=1$ and goes to a finite value for a degenerate ground state ($g_S>1$). In principle, one could use any system with $g_S>1$ and for a large bath $D\to+\infty$ at very low-temperature measure $\mathscr{E}(\delta^2)$ in the system and from that deduce the degeneracy g_E of the ground state of the bath.

We also have $\mathscr{O}((\Delta b)^2\{x_{j,q}\})=0$. Putting everything together with the $(\Delta b)^2$ term gives our final perturbation expression,

$$\begin{aligned}
\mathscr{E}(\delta^2)=&\frac{D}{D+1}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-2\frac{Z_S(3\beta)}{Z_S^3(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]+\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left\{\frac{1}{4k_B\beta^2}C_v^{(S)}(2\beta)+[\langle E(2\beta)\rangle_S-\langle E(\beta)\rangle_S]^2\right\}(\Delta b)^2\\
&+\mathscr{O}((\Delta b)^3)+\mathscr{O}((\Delta b)\{x_{j,q}\}\{x_{j',q'}\})+\mathscr{O}(\{x_{j,q}\}\{x_{j',q'}\}\{x_{j'',q''}\}).
\end{aligned}\tag{B82}$$

Equation (B82) is written as Eq. (29) in the main text, but is written in terms of free energies rather than partition functions.

9. Derivation of $\mathscr{E}(2\sigma^2)$ for the uncoupled entirety

In this section we derive the result for $\mathscr{E}(2\sigma^2)$, starting from the general expression of Eq. (B39) and the definition

$$\sigma = \sqrt{\sum_{i=1}^{D_S-1} \sum_{j=i+1}^{D_S} |\widetilde{\rho}_{i,j}|^2}, \tag{B83}$$

which can be rewritten as

$$\sigma^2 = \frac{1}{2} \sum_{i=1}^{D_S} \sum_{j=1}^{D_S} (1 - \delta_{i,j}) |\widetilde{\rho}_{i,j}|^2. \tag{B84}$$

To second order one has the expression for $2\sigma^2$,

$$\begin{aligned} \mathscr{E}(f_{2\sigma^2}) = {} & \mathscr{E}\left(f_{2\sigma^2}\big|_{\{x\}=\frac{1}{D}}\right) + \frac{1}{2!}\mathscr{E}\left(\left(x - \frac{1}{D}\right)^2\right) \sum_{k=1}^{D_S} \sum_{q=1}^{D_E} \frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}} \\ & + \frac{1}{2!}\mathscr{E}\left(\left(x - \frac{1}{D}\right)\left(x' - \frac{1}{D}\right)\right) \sum_{k=1}^{D_S} \sum_{k'=1}^{D_S} \sum_{q=1}^{D_E} \sum_{q'=1}^{D_E} (1 - \delta_{k,k'}\delta_{q,q'}) \frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q} x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}} \end{aligned} \tag{B85}$$

so there are three terms to calculate. The expectation value involves a sum over all $\phi_{j,p}$ and hence ample use will be made of the properties of Eq. (B28).

We want to calculate without any approximations

$$\mathscr{E}(2\sigma^2) = \mathscr{E}\left(\sum_{j=1}^{D_S} \sum_{j'=1}^{D_S} (1 - \delta_{j,j'}) \widetilde{\rho}^{*}_{j,j'} \widetilde{\rho}_{j,j'} \right). \tag{B86}$$

Let

$$d_{j,p} => \sqrt{x_{j,p}} e^{i\phi_{j,p}} \quad \text{and} \quad d^{*}_{j,p} => \sqrt{x_{j,p}} e^{-i\phi_{j,p}}. \tag{B87}$$

For the case with $\lambda = 0$, the reduced density matrix is

$$\widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\}) = \sum_{p=1}^{D_E} \left\langle E_j^{(S)} \middle| \left\langle E_p^{(E)} \middle| \Psi_\beta \right\rangle \left\langle \Psi_\beta \middle| E_p^{(E)} \right\rangle \middle| E_{j'}^{(S)} \right\rangle = \sum_{p=1}^{D_E} \frac{\sqrt{x_{j,p}}\sqrt{x_{j',p}} e^{i\phi_{j,p}} e^{-i\phi_{j',p}} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_p^{(E)}}{\sum_{j''=1}^{D_S} \sum_{p''=1}^{D_E} x_{j'',p''} p_{j''}^{(S)} p_{p''}^{(E)}}. \tag{B88}$$

The complex conjugate (not the adjoint) is

$$\widetilde{\rho}^{*}_{j,j'}(\beta,\{x\},\{\phi\}) = \sum_{p'=1}^{D_E} \frac{\sqrt{x_{j,p'}}\sqrt{x_{j',p'}} e^{-i\phi_{j,p'}} e^{i\phi_{j',p'}} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_{p'}^{(E)}}{\sum_{j'''=1}^{D_S} \sum_{p'''=1}^{D_E} x_{j''',p'''} p_{j'''}^{(S)} p_{p'''}^{(E)}}. \tag{B89}$$

Extreme care must be taken that both for $x_{j,p}$, $x_{j',p}$, and $x_{j'',p''}$, as well as for $\phi_{j,p}$ and $\phi_{j',p}$, wherever the indices are the same the value of the variable is the same. For example, the value of $x_{3,13}$ is the same in both the numerator and denominator.

a. *Zeroth-order term of $\mathscr{E}(2\sigma^2)$*

We expand about all $x_{j,p} = \frac{1}{D}$, but will perform the exact average over all $\phi_{j,p}$.

The reduced density matrix evaluated at the expansion point $\{x\} = \frac{1}{D}$ is

$$\widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})|_{\{x\}=\frac{1}{D}} = \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} \sum_{p=1}^{D_E} e^{i\phi_{j,p}} e^{-i\phi_{j',p}} p_p^{(E)}. \tag{B90}$$

Similarly, the zeroth-order term also uses the complex conjugate, which is

$$\widetilde{\rho}_{j,j'}(\beta,\{x\},\{-\phi\})|_{\{x\}=\frac{1}{D}} = \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} \sum_{p=1}^{D_E} e^{-i\phi_{j,p}} e^{i\phi_{j',p}} p_p^{(E)}. \tag{B91}$$

The zeroth-order equation is given by

$$\begin{aligned}
f_{2\sigma^2}(\{x\},\{\phi\})|_{\{x\}=\frac{1}{D}} &= \left[\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})\widetilde{\rho}^{*}_{j,j'}(\beta,\{x\},\{\phi\})\widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})\right]\Bigg|_{\{x\}=\frac{1}{D}}\\
&= \left[\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})\frac{\left(\sum_{p=1}^{D_E}\frac{1}{D}e^{-i\phi_{j,p}}e^{i\phi_{j',p}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_p^{(E)}\right)\left(\sum_{p'=1}^{D_E}\frac{1}{D}e^{-i\phi_{j,p'}}e^{i\phi_{j',p'}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_{p'}^{(E)}\right)}{\left(\sum_{j''=1}^{D_S}\sum_{p''=1}^{D_E}\frac{1}{D}p_{j''}^{(S)}p_{p''}^{(E)}\right)^2}\right]\\
&= \sum_{p=1}^{D_E}\sum_{p'=1}^{D_E}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}p_p^{(E)}p_{p'}^{(E)}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}e^{-i\phi_{j,p'}}e^{i\phi_{j',p'}}\\
&= \sum_{p=1}^{D_E}\sum_{p'=1}^{D_E}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}p_p^{(E)}p_{p'}^{(E)}\delta_{p,p'}\delta_{p,p'}\\
&= \left[\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}\right]\left[\sum_{p=1}^{D_E}\left(p_p^{(E)}\right)^2\right] = \left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right],
\end{aligned} \tag{B92}$$

since $\sum_{p=1}^{D_E}p_p^{(E)}=1$ and $\sum_{j=1}^{D_S}p_j^{(S)}=1$. Use has been made of Eq. (B27) with

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{i(\phi_{j,p}-\phi_{j,p'})}d\phi=\delta_{p,p'}, \tag{B93}$$

since

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{i\phi}d\phi=\frac{1}{2\pi i}e^{i\phi}\Big|_{\phi=-\pi}^{\pi}=\frac{1}{2\pi i}(e^{i\pi}-e^{-i\pi})=0. \tag{B94}$$

In the limits one has

$$\begin{aligned}
f_{2\sigma^2}(\{x\},\{\phi\})|_{\{x\}=\frac{1}{D}} &\to \frac{1}{D_E}\frac{D_S-1}{D_S} \qquad \beta\to 0,\\
f_{2\sigma^2}(\{x\},\{\phi\})|_{\{x\}=\frac{1}{D}} &\to \frac{g_S-1}{g_Sg_E} \qquad \beta\to +\infty,
\end{aligned} \tag{B95}$$

where g_S and g_E are the degeneracy of the ground state of H_S and H_E, respectively.

b. First-order term of $\mathscr{E}(2\sigma^2)$

The first partial derivative of $\widetilde{\rho}$ with respect to $x_{k,q}$ is

$$\begin{aligned}
&(1-\delta_{j,j'})\frac{\partial\widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})}{\partial x_{k,q}}\\
&= (1-\delta_{j,j'})\left[\frac{\frac{1}{2}\frac{1}{\sqrt{x_{j,q}}}\sqrt{x_{j',q}}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}}{\sum_{j''=1}^{D_S}\sum_{p''=1}^{D_E}x_{j'',p''}p_{j''}^{(S)}p_{p''}^{(E)}}\delta_{k,j}+\frac{\frac{1}{2}\sqrt{x_{j,q}}\frac{1}{\sqrt{x_{j',q}}}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}}{\sum_{j''=1}^{D_S}\sum_{p''=1}^{D_E}x_{j'',p''}p_{j''}^{(S)}p_{p''}^{(E)}}\delta_{k,j'}\right.\\
&\left.\quad -\frac{p_k^{(S)}p_q^{(E)}\left(\sum_{p=1}^{D_E}\sqrt{x_{j,p}}\sqrt{x_{j',p}}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_p^{(E)}\right)}{\left(\sum_{j''=1}^{D_S}\sum_{p''=1}^{D_E}x_{j'',p''}p_{j''}^{(S)}p_{p''}^{(E)}\right)^2}\right]
\end{aligned} \tag{B96}$$

and evaluating about the expansion point $\{x\} = \frac{1}{D}$ gives

$$
\begin{aligned}
&(1-\delta_{j,j'})\frac{\partial \widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})}{\partial x_{k,q}}\bigg|_{\{x\}=\frac{1}{D}} \\
&= (1-\delta_{j,j'})\Bigg[\frac{D}{2}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j}e^{i\phi_{j,q}}e^{-i\phi_{j',q}} + \frac{D}{2}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j'}e^{i\phi_{j,q}}e^{-i\phi_{j',q}} \\
&\quad - Dp_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}p_p^{(E)}\right)\Bigg] \\
&= (1-\delta_{j,j'})\Bigg[\frac{D}{2}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'}) - Dp_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}p_p^{(E)}\right)\Bigg]. \qquad \text{(B97)}
\end{aligned}
$$

c. Second-order (same) term of $\mathscr{E}(2\sigma^2)$

The second partial derivative with respect to the same $x_{k,q}$, evaluated about $\{x\} = \frac{1}{D}$, is

$$
\begin{aligned}
&(1-\delta_{j,j'})\frac{\partial^2 \widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}} \\
&= (1-\delta_{j,j'})\Bigg[-\frac{D^2}{4}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j} - \frac{D^2}{2}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\big(p_j^{(S)}\big)^{\frac{3}{2}}\sqrt{p_{j'}^{(S)}}\big(p_q^{(E)}\big)^2\delta_{k,j} \\
&\quad -\frac{D^2}{4}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j'} - \frac{D^2}{2}\sqrt{p_j^{(S)}}\big(p_{j'}^{(S)}\big)^{\frac{3}{2}}\big(p_q^{(E)}\big)^2e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j'} \\
&\quad -\frac{D^2}{2}p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\big(p_q^{(E)}\big)^2e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'}) + 2D^2\big(p_k^{(S)}\big)^2\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\big(p_q^{(E)}\big)^2\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}p_p^{(E)}\right)\Bigg].
\end{aligned}
\tag{B98}
$$

One needs to sum over all possible derivatives. Putting together this for the same-$x_{k,q}$ second derivatives gives

$$
\begin{aligned}
\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{q=1}^{D_E}\frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}} &= \frac{1}{2!}\sum_{k=1}^{D_S}\sum_{q=1}^{D_E}\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\Bigg[\frac{\partial^2\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}^2}\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)\bigg|_{\{x\}=\frac{1}{D}} \\
&\quad + 2\frac{\partial\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}}\frac{\partial\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k,q}}\bigg|_{\{x\}=\frac{1}{D}} \\
&\quad + \widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)\frac{\partial^2\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}}\Bigg].
\end{aligned}
\tag{B99}
$$

The first term to calculate for the same-$x_{k,q}$ is

$$
\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{q=1}^{D_E}\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\frac{\partial^2\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}}\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)|_{\{x\}=\frac{1}{D}} \\
&= \frac{1}{2!}\sum_{k=1}^{D_S}\sum_{q=1}^{D_E}\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\left[\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\sum_{p=1}^{D_E}e^{-i\phi_{j,p}}e^{i\phi_{j',p}}p_p^{(E)}\right] \\
&\quad \times\Bigg[-\frac{D^2}{4}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j} - \frac{D^2}{2}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\big(p_j^{(S)}\big)^{\frac{3}{2}}\sqrt{p_{j'}^{(S)}}\big(p_q^{(E)}\big)^2\delta_{k,j} \\
&\quad -\frac{D^2}{4}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\delta_{k,j'} - \frac{D^2}{2}\sqrt{p_j^{(S)}}\big(p_{j'}^{(S)}\big)^{\frac{3}{2}}\big(p_q^{(E)}\big)^2e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j'}
\end{aligned}
$$

$$
\begin{aligned}
&\quad - \frac{D^2}{2} p_k^{(S)} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} \big(p_q^{(E)}\big)^2 e^{i\phi_{j,q}} e^{-i\phi_{j',q}} (\delta_{k,j} + \delta_{k,j'}) + 2D^2 \big(p_k^{(S)}\big)^2 \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} \big(p_q^{(E)}\big)^2 \left(\sum_{p=1}^{D_E} e^{i\phi_{j,p}} e^{-i\phi_{j',p}} p_p^{(E)} \right) \Bigg] \\
&= -\frac{D^2}{8} \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^2 \delta_{k,j} - \frac{D^2}{4} \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) \big(p_j^{(S)}\big)^2 p_{j'}^{(S)} \big(p_q^{(E)}\big)^3 \delta_{k,j} \\
&\quad - \frac{D^2}{8} \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^2 \delta_{k,j'} - \frac{D^2}{4} \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) p_j^{(S)} \big(p_{j'}^{(S)}\big)^2 \big(p_q^{(E)}\big)^3 \delta_{k,j'} \\
&\quad - \frac{D^2}{4} \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) p_k^{(S)} p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^3 (\delta_{k,j} + \delta_{k,j'}) + D^2 \sum_{k,j,j'}^{D_S} \sum_{q=1}^{D_E} (1-\delta_{j,j'}) \big(p_k^{(S)}\big)^2 p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^2 \left\{ \sum_{p'=1}^{D_E} \big[p_{p'}^{(E)}\big]^2 \right\} \\
&= -\frac{D^2}{8} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] - \frac{D^2}{4} \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] - \frac{D^2}{8} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] \\
&\quad - \frac{D^2}{4} \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] - \frac{D^2}{2} \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right] \\
&= -\frac{D^2}{4} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] - D^2 \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right],
\end{aligned} \tag{B100}
$$

and the middle term to calculate is

$$
\begin{aligned}
&\frac{1}{2!} \sum_{k=1}^{D_S} \sum_{q=1}^{D_E} \sum_{j,j'}^{D_S} (1-\delta_{j,j'}) \times 2 \left. \frac{\partial \widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}} \right|_{\{x\}=\frac{1}{D}} \left. \frac{\partial \widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k,q}} \right|_{\{x\}=\frac{1}{D}} \\
&= \sum_{k=1}^{D_S} \sum_{q=1}^{D_E} \sum_{j,j'} (1-\delta_{j,j'}) \left[\frac{D}{2} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_q^{(E)} e^{i\phi_{j,q}} e^{-i\phi_{j',q}} (\delta_{k,j} + \delta_{k,j'}) - D p_k^{(S)} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_q^{(E)} \left(\sum_{p=1}^{D_E} e^{i\phi_{j,p}} e^{-i\phi_{j',p}} p_p^{(E)} \right) \right] \\
&\quad \times \left[\frac{D}{2} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_q^{(E)} e^{-i\phi_{j,q}} e^{i\phi_{j',q}} (\delta_{k,j} + \delta_{k,j'}) - D p_k^{(S)} \sqrt{p_j^{(S)}} \sqrt{p_{j'}^{(S)}} p_q^{(E)} \left(\sum_{p'=1}^{D_E} e^{-i\phi_{j,p'}} e^{i\phi_{j',p'}} p_{p'}^{(E)} \right) \right] \\
&= \frac{D^2}{4} \sum_{k,j,j'}^{D_S} (1-\delta_{j,j'}) \sum_{q=1}^{D_E} p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^2 (\delta_{k,j} + \delta_{k,j'}) - D^2 \sum_{k,j,j'}^{D_S} (1-\delta_{j,j'}) \sum_{q=1}^{D_E} p_k^{(S)} p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^3 (\delta_{k,j} + \delta_{k,j'}) \\
&\quad + D^2 \sum_{k,j,j'}^{D_S} (1-\delta_{j,j'}) \sum_{q=1}^{D_E} \big(p_k^{(S)}\big)^2 p_j^{(S)} p_{j'}^{(S)} \big(p_q^{(E)}\big)^2 \left[\sum_{p=1}^{D_E} \big(p_p^{(E)}\big)^2 \right] \\
&= \frac{D^2}{2} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] - 2D^2 \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right].
\end{aligned} \tag{B101}
$$

Putting this all together for the same $x_{k,q}$ gives

$$
\begin{aligned}
&\frac{1}{2!} \sum_{k=1}^{D_S} \sum_{q=1}^{D_E} \left. \frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}^2} \right|_{\{x\}=\frac{1}{D}} \\
&= -\frac{D^2}{2} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] - 2D^2 \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + 2D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right] \\
&\quad + \frac{D^2}{2} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left[1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right] - 2D^2 \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right] \\
&= -4D^2 \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right] + 3D^2 \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right].
\end{aligned} \tag{B102}
$$

d. Second-order (different) term of $\mathscr{E}(2\sigma^2)$

The different-$x_{k,q}$ second partial derivatives, evaluated about $\{x\} = \frac{1}{D}$ is

$$
\begin{aligned}
&(1-\delta_{j,j'})(1-\delta_{k,k'}\delta_{q,q'})\frac{\partial^2\widetilde{\rho}_{j,j'}(\beta,\{x\},\{\phi\})}{\partial x_{k,q}\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\\
&= (1-\delta_{j,j'})(1-\delta_{k,k'}\delta_{q,q'})\Bigg[\frac{D^2}{4}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j}\delta_{k',j'}\delta_{q,q'} - \frac{D^2}{2}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j}\\
&\quad + \frac{D^2}{4}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j'}\delta_{k',j}\delta_{q,q'} - \frac{D^2}{2}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}\delta_{k,j'}\\
&\quad - \frac{D^2}{2}p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q'}}e^{-i\phi_{j',q'}}\delta_{k',j} - \frac{D^2}{2}p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q'}}e^{-i\phi_{j',q'}}\delta_{k',j'}\\
&\quad + 2D^2\,p_k^{(S)}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}p_p^{(E)}\right)\Bigg]\\
&= (1-\delta_{j,j'})(1-\delta_{k,k'}\delta_{q,q'})\Bigg[\frac{D^2}{4}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j})\delta_{q,q'}\\
&\quad - \frac{D^2}{2}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'}) - \frac{D^2}{2}p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k',j}+\delta_{k',j'})\\
&\quad + 2D^2\,p_k^{(S)}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}p_q^{(E)}p_{q'}^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}p_p^{(E)}\right)\Bigg],
\end{aligned}
\tag{B103}
$$

where the terms have been combined.

One needs to sum over all possible derivatives. Putting together this for the different-$x_{k,q}$ second derivatives gives

$$
\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\\
&= \frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\frac{\partial^2[\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)]}{\partial x_{k,q}\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\\
&= \frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\Bigg[\frac{\partial^2\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}\partial x_{k',q'}}\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)\bigg|_{\{x\}=\frac{1}{D}}\\
&\quad + \frac{\partial\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}}\frac{\partial\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\\
&\quad + \frac{\partial\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k',q'}}\frac{\partial\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k,q}}\bigg|_{\{x\}=\frac{1}{D}}\\
&\quad + \widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)\frac{\partial^2\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k,q}\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\Bigg].
\end{aligned}
\tag{B104}
$$

We need to sum over all possible derivatives. The first term to analyze for different-$x_{k,q}$ is

$$
\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}(1-\delta_{j,j'})\frac{\partial^2\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}\partial x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)|_{\{x\}=\frac{1}{D}}\\
&= \frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\left[\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\left(\sum_{p'=1}^{D_E}e^{-i\phi_{j,p'}}e^{i\phi_{j',p'}}p_{p'}^{(E)}\right)\right]
\end{aligned}
$$

$$\begin{aligned}
&\times\Bigg[\frac{D^2}{4}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j})\delta_{q,q'}-\frac{D^2}{2}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'})\\
&-\frac{D^2}{2}p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k',j}+\delta_{k',j'})+2D^2\,p_k^{(S)}p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}p_{q'}^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}\,p_p^{(E)}\right)\Bigg]\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}\left[\sum_{p'=1}^{D_E}e^{-i\phi_{j,p'}}e^{i\phi_{j',p'}}\,p_{p'}^{(E)}\right]\\
&\times\Bigg[\frac{D^2}{4}p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j})\delta_{q,q'}-\frac{D^2}{2}p_{k'}^{(S)}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'})\\
&-\frac{D^2}{2}p_k^{(S)}p_q^{(E)}p_{q'}^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k',j}+\delta_{k',j'})+2D^2\,p_k^{(S)}p_{k'}^{(S)}p_q^{(E)}p_{q'}^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}\,p_p^{(E)}\right)\Bigg]\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}\Bigg\{\frac{D^2}{4}\big(p_q^{(E)}\big)^2(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j})\delta_{q,q'}\\
&-\frac{D^2}{2}p_{k'}^{(S)}\big(p_q^{(E)}\big)^2p_{q'}^{(E)}(\delta_{k,j}+\delta_{k,j'})-\frac{D^2}{2}p_k^{(S)}\big(p_q^{(E)}\big)^2p_{q'}^{(E)}(\delta_{k',j}+\delta_{k',j'})+2D^2\,p_k^{(S)}p_{k'}^{(S)}p_q^{(E)}p_{q'}^{(E)}\left[\sum_{p=1}^{D_E}\big(p_p^{(E)}\big)^2\right]\Bigg\}\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}\Bigg\{\frac{D^2}{4}(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j})(1-\delta_{k,k'})\frac{Z_E(2\beta)}{Z_E^2(\beta)}\\
&-\frac{D^2}{2}p_{k'}^{(S)}(\delta_{k,j}+\delta_{k,j'})\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]-\frac{D^2}{2}p_k^{(S)}(\delta_{k',j}+\delta_{k',j'})\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&+2D^2\,p_k^{(S)}p_{k'}^{(S)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\},
\end{aligned}\tag{B105}$$

which multiplying out gives

$$\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}(1-\delta_{j,j'})\left.\frac{\partial^2\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}\partial x_{k',q'}}\right|_{\{x\}=\frac{1}{D}}\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)|_{\{x\}=\frac{1}{D}}\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}p_j^{(S)}p_{j'}^{(S)}\Bigg\{\frac{D^2}{4}(\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j}-\delta_{j,j'}\delta_{k,j}\delta_{k',j'}-\delta_{j,j'}\delta_{k,j'}\delta_{k',j}\\
&\quad-\delta_{k,k'}\delta_{k,j}\delta_{k',j'}-\delta_{k,k'}\delta_{k,j'}\delta_{k',j}+\delta_{k,k'}\delta_{j,j'}\delta_{k,j}\delta_{k',j'}+\delta_{k,k'}\delta_{j,j'}\delta_{k,j'}\delta_{k',j})\frac{Z_E(2\beta)}{Z_E^2(\beta)}\\
&\quad-\frac{D^2}{2}p_{k'}^{(S)}\bigg[\delta_{k,j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\delta_{k,j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\\
&\quad-\delta_{j,j'}\delta_{k,j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k,j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\delta_{j,j'}\delta_{k,j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k,j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\bigg]\\
&\quad-\frac{D^2}{2}p_k^{(S)}\bigg[\delta_{k',j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k',j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\delta_{k',j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k',j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\\
&\quad-\delta_{j,j'}\delta_{k',j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k',j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\delta_{j,j'}\delta_{k',j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k',j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\bigg]
\end{aligned}$$

$$
\begin{aligned}
&+2D^2\, p_k^{(S)} p_{k'}^{(S)} \frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\delta_{j,j'}-\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\}\\
&=\Bigg\{\frac{D^2}{8}\left[1+1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}+\frac{Z_S(2\beta)}{Z_S^2(\beta)}+\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\frac{Z_E(2\beta)}{Z_E^2(\beta)}\\
&-\frac{D^2}{4}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&-\frac{D^2}{4}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&+D^2\,\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\}\\
&=D^2\Bigg\{\frac{1}{4}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&+\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\}\\
&=\frac{D^2}{4}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]+D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right],
\end{aligned}
\tag{B106}
$$

which is not too pretty of an expression.

The second term (first middle term) to calculate is

$$
\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\left.\frac{\partial\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}}\right|_{\{x\}=\frac{1}{D}}\left.\frac{\partial\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k',q'}}\right|_{\{x\}=\frac{1}{D}}\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}\sum_{j,j'}^{D_S}(1-\delta_{k,k'}\delta_{q,q'})(1-\delta_{j,j'})\left[\frac{D}{2}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}e^{i\phi_{j,q}}e^{-i\phi_{j',q}}(\delta_{k,j}+\delta_{k,j'})\right.\\
&\left.-D\,p_k^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_q^{(E)}\left(\sum_{p=1}^{D_E}e^{i\phi_{j,p}}e^{-i\phi_{j',p}}\,p_p^{(E)}\right)\right]\left[\frac{D}{2}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_{q'}^{(E)}e^{-i\phi_{j,q'}}e^{i\phi_{j',q'}}(\delta_{k',j}+\delta_{k',j'})\right.\\
&\left.-D\,p_{k'}^{(S)}\sqrt{p_j^{(S)}}\sqrt{p_{j'}^{(S)}}\,p_{q'}^{(E)}\left(\sum_{p'=1}^{D_E}e^{-i\phi_{j,p'}}e^{i\phi_{j',p'}}\,p_{p'}^{(E)}\right)\right]\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{k,k'}\delta_{q,q'})(1-\delta_{j,j'})\Bigg\{\frac{D^2}{4}p_j^{(S)}p_{j'}^{(S)}p_q^{(E)}p_{q'}^{(E)}\delta_{q,q'}(\delta_{k,j}+\delta_{k,j'})(\delta_{k',j}+\delta_{k',j'})\\
&-\frac{D^2}{2}p_{k'}^{(S)}p_j^{(S)}p_{j'}^{(S)}\big(p_q^{(E)}\big)^2p_{q'}^{(E)}(\delta_{k,j}+\delta_{k,j'})-\frac{D^2}{2}p_k^{(S)}p_j^{(S)}p_{j'}^{(S)}p_q^{(E)}\big(p_{q'}^{(E)}\big)^2(\delta_{k',j}+\delta_{k',j'})\\
&+D^2p_k^{(S)}p_{k'}^{(S)}p_j^{(S)}p_{j'}^{(S)}p_q^{(E)}p_{q'}^{(E)}\left[\sum_{p=1}^{D_E}\big(p_p^{(E)}\big)^2\right]\Bigg\}\\
&=\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S}(1-\delta_{j,j'})p_j^{(S)}p_{j'}^{(S)}\Bigg\{\frac{D^2}{4}\frac{Z_E(2\beta)}{Z_E^2(\beta)}(\delta_{k,j}+\delta_{k,j'})(\delta_{k',j}+\delta_{k',j'})(1-\delta_{k,k'})\\
&-\frac{D^2}{2}p_{k'}^{(S)}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right](\delta_{k,j}+\delta_{k,j'})-\frac{D^2}{2}p_k^{(S)}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right](\delta_{k',j}+\delta_{k',j'})
\end{aligned}
$$

$$\begin{aligned}
&+D^2 p_k^{(S)} p_{k'}^{(S)}\left[1-\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\}\\
&=\frac{D^2}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{j=1}^{D_S}\sum_{j'=1}^{D_S} p_j^{(S)} p_{j'}^{(S)}\Bigg\{\frac{1}{4}\frac{Z_E(2\beta)}{Z_E^2(\beta)}(\delta_{k,j}\delta_{k',j}+\delta_{k,j'}\delta_{k',j}+\delta_{k,j}\delta_{k',j'}+\delta_{k,j'}\delta_{k',j'})(1-\delta_{k,k'}-\delta_{j,j'}+\delta_{k,k'}\delta_{j,j'})\\
&-\frac{1}{2}p_{k'}^{(S)}\left[\delta_{k,j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\delta_{k,j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k,j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\delta_{j,j'}\delta_{k,j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k,j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\delta_{j,j'}\delta_{k,j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k,j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&-\frac{1}{2}p_{k}^{(S)}\left[\delta_{k',j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k',j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\delta_{k',j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{k',j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\delta_{j,j'}\delta_{k',j}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k',j}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\delta_{j,j'}\delta_{k',j'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\delta_{j,j'}\delta_{k',j'}\delta_{k,k'}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&+p_k^{(S)}p_{k'}^{(S)}\left[1-\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\delta_{j,j'}+\delta_{j,j'}\delta_{k,k'}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\},
\end{aligned}\tag{B107}$$

which is simplified to

$$\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\sum_{j,j'}^{D_S}(1-\delta_{j,j'})\left.\frac{\partial\widetilde{\rho}(\{x\},\phi_1,\phi_2,\ldots,\phi_D)}{\partial x_{k,q}}\right|_{\{x\}=\frac{1}{D}}\left.\frac{\partial\widetilde{\rho}(\{x\},-\phi_1,-\phi_2,\ldots,-\phi_D)}{\partial x_{k',q'}}\right|_{\{x\}=\frac{1}{D}}\\
&=\frac{D^2}{2!}\Bigg\{\frac{1}{2}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]-\frac{1}{2}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&-\frac{1}{2}\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right.\\
&\left.-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\right]\\
&+\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\left[\frac{Z_E(2\beta)}{Z_E^2(\beta)}\right]\Bigg\}\\
&=\frac{D^2}{2!}\Bigg\{\frac{1}{2}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]-\frac{Z_E(2\beta)}{Z_E^2(\beta)}+2\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}+\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\\
&+2\frac{Z_S(3\beta)}{Z_S^3(\beta)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}+\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\Bigg\}\\
&=-\frac{D^2}{4}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]+D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-\frac{D^2}{2}\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right],
\end{aligned}\tag{B108}$$

which is also not a pretty expression.

The last two terms give the same results as the first two, since they are complex conjugates of the first two terms. For example, the fourth term is the complex conjugate of the first term, and the result after the averaging over the $\{\phi\}$ is real, so the final result for the fourth term equals the final result for the first term.

Collecting the four terms gives the final result for the different-$x_{k,q}$ second derivatives to be

$$\begin{aligned}
&\frac{1}{2!}\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\left.\frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}\partial x_{k',q'}}\right|_{\{x\}=\frac{1}{D}}\\
&=\frac{D^2}{2}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]+2D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]
\end{aligned}$$

$$
\begin{aligned}
&-2D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]-\frac{D^2}{2}\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\\
&+2D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}+\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\\
=\;&4D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-3D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right],
\end{aligned}
\tag{B109}
$$

which is the same as the same-$x_{k,q}$ term except for a negative sign.

e. $0th$*,* $1st$*, and* $2nd$ *terms of* $\mathscr{E}(2\sigma^2)$

To second order one has the final expression for $2\sigma^2$, now that all $\phi_{k,q}$ have correctly been taken into account,

$$
\begin{aligned}
\mathscr{E}(f_{2\sigma^2}) =\;& \mathscr{E}\left(f_{2\sigma^2}\big|_{\{x\}=\frac{1}{D}}\right)+\frac{1}{2!}\mathscr{E}\left(\left(x-\frac{1}{D}\right)^2\right)\sum_{k=1}^{D_S}\sum_{q=1}^{D_E}\frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}^2}\bigg|_{\{x\}=\frac{1}{D}}\\
&+\frac{1}{2!}\mathscr{E}\left(\left(x-\frac{1}{D}\right)\left(x'-\frac{1}{D}\right)\right)\sum_{k=1}^{D_S}\sum_{k'=1}^{D_S}\sum_{q=1}^{D_E}\sum_{q'=1}^{D_E}(1-\delta_{k,k'}\delta_{q,q'})\frac{\partial^2 f_{2\sigma^2}}{\partial x_{k,q}x_{k',q'}}\bigg|_{\{x\}=\frac{1}{D}}\\
=\;&\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]+\left[\frac{D-1}{D^2(D+1)}\right]\left\{-4D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]+3D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\\
&+\left[-\frac{1}{D^2(D+1)}\right]\left\{4D^2\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-3D^2\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\right\}\\
=\;&\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]+\left[\frac{D-1}{(D+1)}\right]\left\{-4\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]+3\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\\
&+\left[-\frac{1}{(D+1)}\right]\left\{4\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]-3\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\frac{Z_S(2\beta)}{Z_S^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]\right\}\\
=\;&\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right]-4\frac{D}{(D+1)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S(3\beta)}{Z_S^3(\beta)}\right]+3\frac{D}{(D+1)}\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)}-\frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right].
\end{aligned}
\tag{B110}
$$

Equation (B110) is written as Eq. (27) in the main text, but is written in terms of free energies rather than partition functions.

In the limit of high temperature ($\beta \to 0$), one has that $Z_E(0) = D_E$ and $Z_S(0) = D_S$ to give

$$
\begin{aligned}
\lim_{\beta\to 0}\mathscr{E}(f_{2\sigma^2}) &= \frac{D_E}{D_E^2}\left(1-\frac{D_S}{D_S^2}\right)-4\frac{D}{D+1}\frac{D_E}{D_E^3}\left(\frac{D_S}{D_S^2}-\frac{D_S}{D_S^3}\right)+3\frac{D}{D+1}\frac{D_E^2}{D_E^4}\left(\frac{D_S}{D_S^2}-\frac{D_S^2}{D_S^4}\right)\\
&= \frac{1}{D_E}\left(1-\frac{1}{D_S}\right)-4\frac{D_E D_S}{D+1}\frac{1}{D_E^2}\left(\frac{1}{D_S}-\frac{1}{D_S^2}\right)+3\frac{D_E D_S}{D+1}\frac{1}{D_E^2}\left(\frac{1}{D_S}-\frac{1}{D_S^2}\right)\\
&= \frac{1}{D_E}\frac{(D_S-1)}{D_S}-\frac{1}{D+1}\frac{1}{D_E}\left(1-\frac{1}{D_S}\right)=\frac{D}{D+1}\frac{1}{D_E}\frac{(D_S-1)}{D_S}=\frac{D_S-1}{D+1}=\frac{D_S-1}{D_E D_S+1}.
\end{aligned}
\tag{B111}
$$

One can perform an expansion about $\beta = 0$ (temperature $T = \infty$). In particular, use that the average internal energy for the environment is given by

$$
\langle E(n\beta)\rangle_E = -\frac{\partial \ln[Z_E(n\beta)]}{\partial(n\beta)} = -\frac{1}{Z_E(n\beta)}\frac{1}{n}\frac{\partial Z_E(n\beta)}{\partial\beta}
\tag{B112}
$$

so

$$
\frac{\partial Z_E(n\beta)}{\partial\beta} = -n\langle E(n\beta)\rangle_E Z_E(n\beta).
\tag{B113}
$$

It is similar for the derivatives of $Z_S(n\beta)$ for the system,

$$
\frac{\partial Z_S(n\beta)}{\partial\beta} = -n\langle E(n\beta)\rangle_S Z_S(n\beta).
\tag{B114}
$$

Taking the limit $\beta = 0$ gives the average internal energy at infinite temperature, $U_\infty^{(E)}$ and $U_\infty^{(S)}$, for the environment and system, respectively. Thus,

$$\left.\frac{\partial Z_S(n\beta)}{\partial\beta}\right|_{\beta=0} = -nU_\infty^{(S)}D_S \quad \text{and} \quad \left.\frac{\partial Z_E(n\beta)}{\partial\beta}\right|_{\beta=0} = -nU_\infty^{(E)}D_E. \tag{B115}$$

Note that

$$\left.\frac{\partial}{\partial\beta}\left[\frac{Z_E^m(n\beta)}{Z_E^{mn}(\beta)}\right]\right|_{\beta=0} = -\frac{nmD_E^{m-1}D_E}{D_E^{mn}}U_\infty^{(E)} + \frac{nmD_E^mD_E}{D_E^{mn+1}}U_\infty^{(E)} = 0 \tag{B116}$$

and similarly for the system Z_S. Thus, the first-order term in the expansion about $\beta = 0$ vanishes. This gives that for small β the Taylor expansion is

$$\mathscr{E}(f_{2\sigma^2}) \approx \frac{D_S - 1}{D_ED_S + 1} + \mathscr{O}(\beta^2). \tag{B117}$$

The second-order terms should be in terms of the heat capacities at constant volume, $C_{E,v}$ and $C_{S,v}$, since

$$C_{S,v} = \frac{\partial\langle E\rangle_S}{\partial T} = k_{\mathrm{B}}\beta^2\frac{\partial\langle E\rangle_S}{\partial\beta} = -k_{\mathrm{B}}\beta^2\frac{\partial^2\ln[Z_S(\beta)]}{\partial\beta^2} = k_{\mathrm{B}}\beta^2\left\{\frac{1}{Z_S(\beta)}\frac{\partial^2 Z_S(\beta)}{\partial\beta^2} - \left[\frac{1}{Z_S(\beta)}\frac{\partial Z_S(\beta)}{\partial\beta}\right]^2\right\}. \tag{B118}$$

In order to calculate more easily the second-order term, define

$$R_E(n_E\beta) = \frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)} \quad \text{and} \quad R_S(n_S\beta) = \frac{Z_S(n_S\beta)}{Z_S^{n_S}(\beta)} \tag{B119}$$

and evaluated at $\beta = 0$ gives

$$R_E(n_E\beta)|_{\beta=0} = \left.\frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)}\right|_{\beta=0} = \frac{D_E}{D_E^{n_E}} = \frac{1}{D_E^{n_E-1}}. \tag{B120}$$

The first derivative is

$$\begin{aligned}\frac{\partial R_E(n_E\beta)}{\partial\beta} &= \frac{\partial}{\partial\beta}\left[\frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)}\right] = \frac{1}{Z_E^{n_E}(\beta)}\frac{\partial Z_E(n_E\beta)}{\partial\beta} - \frac{n_EZ_E(n_E\beta)}{Z_E^{n_E+1}(\beta)}\frac{\partial Z_E(\beta)}{\partial\beta}\\ &= -\frac{n_EZ_E(n_E\beta)}{Z_E^{n_E}(\beta)}\langle E(n_E\beta)\rangle_E + \frac{n_EZ_E(n_E\beta)}{Z_E^{n_E}(\beta)}\langle E(\beta)\rangle_E\end{aligned} \tag{B121}$$

and evaluated at $\beta = 0$ gives

$$\begin{aligned}\left.\frac{\partial R_E(n_E\beta)}{\partial\beta}\right|_{\beta=0} &= \left.\frac{\partial}{\partial\beta}\left[\frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)}\right]\right|_{\beta=0}\\ &= -\frac{n_EZ_E(n_E\beta)}{Z_E^{n_E}(\beta)}\langle E(n_E\beta)\rangle_E\Big|_{\beta=0} + \frac{n_EZ_E(n_E\beta)}{Z_E^{n_E}(\beta)}\langle E(\beta)\rangle_E\Big|_{\beta=0} = -\frac{n_ED_E}{D_E^{n_E}}U_\infty^{(E)} + \frac{n_ED_E}{D_E^{n_E}}U_\infty^{(E)} = 0.\end{aligned} \tag{B122}$$

The second-order derivative is

$$\begin{aligned}\frac{\partial^2 R_E(n_E\beta)}{\partial\beta^2} &= \frac{\partial^2}{\partial\beta^2}\left[\frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)}\right] = \frac{1}{Z_E^{n_E}(\beta)}\frac{\partial^2 Z_E(n_E\beta)}{\partial\beta^2} - n_E\frac{1}{Z_E^{n_E+1}(\beta)}\frac{\partial Z_E(n_E\beta)}{\partial\beta}\frac{\partial Z_E(\beta)}{\partial\beta}\\ &\quad - \frac{n_EZ_E(n_E\beta)}{Z_E^{n_E+1}(\beta)}\frac{\partial^2 Z_E(\beta)}{\partial\beta^2} - \frac{n_E}{Z_E^{n_E+1}(\beta)}\frac{\partial Z_E(\beta)}{\partial\beta}\frac{\partial Z_E(n_E\beta)}{\partial\beta} + \frac{n_E(n_E+1)Z_E(n_E\beta)}{Z_E^{n_E+2}(\beta)}\left[\frac{\partial Z_E(\beta)}{\partial\beta}\right]^2,\end{aligned} \tag{B123}$$

or using the definition of the specific heat as

$$\frac{\partial^2 Z_E(n_E\beta)}{\partial\beta^2} = -\frac{1}{k_{\mathrm{B}}\beta^2}Z_E(n_E\beta)C_{E,v}(n_E\beta), \tag{B124}$$

with the limiting result

$$\left.\frac{\partial^2 Z_E(n_E\beta)}{\partial\beta^2}\right|_{\beta=0} = -\frac{n_E}{k_{\mathrm{B}}\beta^2}Z_E(n_E\beta)C_{E,v}(n_E\beta)\Big|_{\beta=0} = -\frac{n_E}{k_{\mathrm{B}}\beta^2}D_EC_{E,v}(\infty), \tag{B125}$$

gives

$$\left.\frac{\partial^2 R_E(n_E\beta)}{\partial\beta^2}\right|_{\beta=0} = \left.\frac{\partial^2}{\partial\beta^2}\left[\frac{Z_E(n_E\beta)}{Z_E^{n_E}(\beta)}\right]\right|_{\beta=0} = \frac{n_E}{D_E^{n_E}}\left(-\frac{1}{k_{\rm B}\beta^2}\right)D_E C_{E,v}(\infty) - \left(\frac{n_E D_E}{D_E^{n_E+1}}\right)\left(-\frac{n_E}{k_{\rm B}\beta^2}\right)D_E C_{E,v}(\infty)$$

$$= \frac{n_E C_{E,v}(\infty)}{k_{\rm B}\beta^2}\left(\frac{n_E}{D_E^{n_E-1}} - \frac{1}{D_E^{n_E-1}}\right) = \frac{n_E(n_E-1)C_{E,v}(\infty)}{k_{\rm B}\beta^2 D_E^{n_E-1}}. \tag{B126}$$

Note that both

$$\left.\frac{\partial R_E(n_E\beta)}{\partial\beta}\right|_{\beta=0} = 0 \quad \text{and} \quad \text{if} \quad n_E = 1\, \left.\frac{\partial R_E(n_E\beta)}{\partial\beta}\right|_{\beta=0,n_E=1} = 0. \tag{B127}$$

These greatly cut down on the number of nonzero terms from Eq. (B110). One has that

$$\frac{\partial^2}{\partial\beta^2}\left\{\frac{Z_E(2\beta)}{Z_E^2(\beta)}\left[1-\frac{Z_S(2\beta)}{Z_S^2(\beta)}\right] - 4\frac{D}{(D+1)}\frac{Z_E(3\beta)}{Z_E^3(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)}\right] + 3\frac{D}{(D+1)}\frac{Z_E^2(2\beta)}{Z_E^4(\beta)}\left[\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)}\right]\right\}\Bigg|_{\beta=0}$$

$$= \frac{2C_{E,v}(\infty)}{k_{\rm B}\beta^2 D_E}\left(1-\frac{1}{D_S}\right) - \frac{1}{D_E}\frac{2C_{S,v}(\infty)}{k_{\rm B}\beta^2 D_S} - 4\frac{D}{D+1}\left[\frac{6C_{E,v}(\infty)}{k_{\rm B}\beta^2 D_E^2}\left(\frac{1}{D_S}-\frac{1}{D_S^2}\right) + \frac{1}{D_E^2}\frac{C_{S,v}(\infty)}{k_{\rm B}\beta^2}\left(\frac{2}{D_S}-\frac{6}{D_S^2}\right)\right]$$

$$+3\frac{D}{D+1}\left[\frac{4C_{E,v}(\infty)}{k_{\rm B}\beta^2 D_E^3}\left(\frac{1}{D_S}-\frac{1}{D_S^2}\right) + \frac{1}{D_E^2}\frac{C_{S,v}(\infty)}{k_{\rm B}\beta^2}\left(\frac{2}{D_S}-\frac{8}{D_S^3}\right)\right]$$

$$= \frac{2C_{E,v}(\infty)(D_S-1)}{k_{\rm B}\beta^2 D} - \frac{1}{D}\frac{2C_{S,v}(\infty)}{k_{\rm B}\beta^2} - 4\frac{1}{D(D+1)}\frac{2}{k_{\rm B}\beta^2}[3C_{E,v}(\infty)(D_S-1) + C_{S,v}(\infty)(D_S-3)]$$

$$+\,3\frac{1}{D(D+1)}\frac{2}{k_{\rm B}\beta^2}\left[\frac{2C_{E,v}(\infty)}{D_E}(D_S-1) + \frac{C_{S,v}(\infty)}{D_S}\left(D_S^2-4\right)\right]$$

$$= \frac{C_{E,v}(\infty)}{Dk_{\rm B}\beta^2}\left[2D_S - 1 - 24\frac{D_S-1}{D+1} + 12\frac{D_S-1}{D_E(D+1)}\right] + \frac{C_{S,v}(\infty)}{Dk_{\rm B}\beta^2}\left[-2 - 8\frac{(D_S-1)}{D+1} + 6\frac{D_S^2-4}{D+1}\right]. \tag{B128}$$

Therefore, the final result to second order about $\beta = 0$ is

$$\mathscr{E}(f_{2\sigma^2}) = \frac{D_S-1}{D+1} + \frac{1}{2!}\beta^2\left\{\frac{C_{E,v}(\infty)}{Dk_{\rm B}\beta^2}\left[2D_S - 1 - 24\frac{D_S-1}{D+1} + 12\frac{D_S-1}{D_E(D+1)}\right] + \frac{2C_{S,v}(\infty)}{Dk_{\rm B}\beta^2}\left[-1 + 2\frac{\left(3D_S^2 - 4D_S - 8\right)}{D+1}\right]\right\}. \tag{B129}$$

One has to be cautious about the low-temperature ($\beta \to +\infty$) limit, since the analysis requires that $\beta\langle H_{SE}\rangle$ be small. Then the partition function can be written as

$$Z_S(n\beta) = e^{-n\beta E_0^{(S)}}\left(g_S + \sum_{j=1}^{D_s-g_S} e^{-n\beta(E_j^{(S)}-E_0^{(S)})}\right) \to_{\beta\to+\infty} g_S e^{-n\beta E_0^{(S)}}. \tag{B130}$$

It is similar for the partition function $Z_E(n\beta)$. Thus, one has

$$\lim_{\beta\to+\infty}\mathscr{E}(f_{2\sigma^2}) = \frac{1}{g_E}\left(1-\frac{1}{g_S}\right) - \frac{D}{D+1}\frac{1}{g_E^2}\left(\frac{1}{g_S}-\frac{1}{g_S^2}\right) = \frac{g_S-1}{g_E g_S}\left[1-\frac{D}{(D+1)g_E g_S}\right]. \tag{B131}$$

This expression goes to zero if the system ground state is nondegenerate. For a highly degenerate system ground state ($g_S \gg 1$) the expression goes to $1/g_E$. Thus, in principle, one could use any system with $g_S > 1$ and for a large bath $D \to +\infty$ at very low-temperature measure $\mathscr{E}(f_{2\sigma^2})$ in the system and from that deduce the degeneracy of the ground state of the bath.

10. Coupled entirety

Our goal is to calculate in perturbation theory the expectation for σ^2, up to first order in the interaction Hamiltonian λH_I in Eq. (B1). We then show that for particular common symmetries this first-order term is zero.

Let us start with a formula from Wilcox (Eq. 4.1 of Ref. [51]) of

$$\frac{\partial e^{H(\lambda)}}{\partial\lambda} = \int_0^1 d\xi\, e^{\xi H(\lambda)}\frac{\partial H(\lambda)}{\partial\lambda}e^{-\xi H(\lambda)}e^{H(\lambda)} \tag{B132}$$

$$= e^{H(\lambda)}\int_0^1 d\xi\, e^{-\xi H(\lambda)}\frac{\partial H(\lambda)}{\partial\lambda}e^{\xi H(\lambda)}. \tag{B133}$$

Then one has

$$
\begin{aligned}
e^{-\beta H} &\approx e^{-\beta H_0} + \left\{\frac{\partial e^{-\beta H_0-\beta\delta H_I}}{\partial\lambda}\right\}\bigg|_{\lambda=0}\lambda = e^{-\beta H_0} + \left\{\int_0^1 d\xi e^{-\beta\xi H}\frac{\partial(-\beta H)}{\partial\lambda}e^{\beta\xi H}e^{-\beta H}\right\}\bigg|_{\lambda=0}\lambda \\
&= \left(1-\left\{\int_0^1 d\xi e^{-\beta\xi H_0}H_I e^{\beta\xi H_0}\right\}\beta\lambda\right)e^{-\beta H_0} \qquad \text{(B134)} \\
&= e^{-\beta H_0}\left(1-\left\{\int_0^1 d\xi e^{\beta\xi H_0}H_I e^{-\beta\xi H_0}\right\}\beta\lambda\right). \qquad \text{(B135)}
\end{aligned}
$$

The wave function we start our dynamics with is given by Eq. (B6). The first-order perturbation comes from both the denominator and numerator of Eq. (B6). First, let us deal with the denominator. Up to the first order, we have

$$
\begin{aligned}
\langle\Psi_0|e^{-\beta H}|\Psi_0\rangle &= \langle\Psi_0|e^{-\beta H_0} - \left\{\int_0^1 d\xi e^{-\beta\xi H_0}H_I e^{\beta\xi H_0}\right\}\beta\lambda e^{-\beta H_0} + \mathscr{O}(\lambda^2)|\Psi_0\rangle \\
&= \langle\Psi_0|e^{-\beta H_0}|\Psi_0\rangle - \beta\lambda\langle\Psi_0|\int_0^1 d\xi e^{-\beta\xi H_0}H_I e^{-\beta(1-\xi)H_0}|\Psi_0\rangle + \mathscr{O}(\lambda^2) \\
&= \langle\Psi_0|e^{-\beta H_0}|\Psi_0\rangle - \beta\lambda\int_0^1 d\xi\langle\Psi_0|e^{-\beta\xi H_0}H_I e^{-\beta(1-\xi)H_0}|\Psi_0\rangle + \mathscr{O}(\lambda^2). \qquad \text{(B136)}
\end{aligned}
$$

According to the results in Ref. [40], for large D we have

$$\mathrm{Tr}A \approx D\langle\Psi_0|A|\Psi_0\rangle, \qquad \text{(B137)}$$

where A is an operator which is acting on a D-dimensional Hilbert space. Then the denominator of Eq. (B6) reads

$$D\langle\Psi_0|e^{-\beta H}|\Psi_0\rangle \approx \mathrm{Tr}e^{-\beta H_0} - \beta\lambda\int_0^1 d\xi\mathrm{Tr}e^{-\beta\xi H_0}H_I e^{-\beta(1-\xi)H_0} = \mathrm{Tr}e^{-\beta H_0} - \beta\lambda\mathrm{Tr}e^{-\beta H_0}H_I. \qquad \text{(B138)}$$

If we restrict the Hamiltonian into the Heisenberg type which is given by

$$
\begin{aligned}
H_S &= -\sum_{i=1}^{N_S-1}\sum_{j=i+1}^{N_S}\sum_{\alpha=x.y,z} J_{i,j}^{\alpha}S_i^{\alpha}S_j^{\alpha}, \qquad \text{(B139)} \\
H_E &= -\sum_{i=1}^{N_E-1}\sum_{j=i+1}^{N_E}\sum_{\alpha=x,y,z} \Omega_{i,j}^{\alpha}I_i^{\alpha}I_j^{\alpha}, \qquad \text{(B140)} \\
H_{SE} &= -\sum_{i=1}^{N_S}\sum_{j=1}^{N_E}\sum_{\alpha=x,y,z} \lambda_{i,j}^{\alpha}S_i^{\alpha}I_j^{\alpha}, \qquad \text{(B141)}
\end{aligned}
$$

where S and I are referring to the spin-$\frac{1}{2}$ operator of the system and environment respectively, then the first-order term of the denominator of Eq. (B6) is zero. To see this, we apply a unitary transformation U which transforms $S \to -S$ and $I \to I$ or $S \to S$ and $I \to -I$ to the first-order term. The transformation does not change the Hamiltonian $H_0 = H_S + H_E$, but changes the Hamiltonian H_I into $-H_I$. One has

$$\mathrm{Tr}e^{-\beta H_0}H_I = \mathrm{Tr}UU^{+}e^{-\beta H_0}UU^{+}H_I = -\mathrm{Tr}e^{-\beta H_0}H_I. \qquad \text{(B142)}$$

Therefore, the first-order term has to be zero.

Now up to the first order, we have

$$\langle\Psi_0|e^{-\beta H}|\Psi_0\rangle \approx \mathrm{Tr}e^{-\beta H_0}/D = Z_0/D, \qquad \text{(B143)}$$

where Z_0 is the partition function of the unperturbed system. Then the wave function is thus given approximately by

$$|\Psi_\beta\rangle \approx \sqrt{\frac{D}{Z_0}}e^{-\beta H/2}|\Psi_0\rangle = \sqrt{\frac{D}{Z_0}}\left[1-\left\{\int_0^1 d\xi e^{-\beta\xi H_0/2}H_I e^{\beta\xi H_0/2}\right\}\beta\lambda/2+\mathscr{O}(\lambda^2)\right]e^{-\beta H_0/2}|\Psi_0\rangle. \qquad \text{(B144)}$$

The corresponding bra is

$$\langle\Psi_\beta| \approx \sqrt{\frac{D}{Z_0}}\langle\Psi(0)|e^{-\beta H/2} = \sqrt{\frac{D}{Z_0}}\langle\Psi(0)|e^{-\beta H_0/2}\left[1-\left\{\int_0^1 d\xi e^{\beta\xi H_0/2}H_I e^{-\beta\xi H_0/2}\right\}\beta\lambda/2+\mathscr{O}(\lambda^2)\right]. \qquad \text{(B145)}$$

The density matrix of the entirety $S+E$ is given by

$$\begin{aligned}\rho &= |\Psi_\beta\rangle\langle\Psi_\beta| \approx \frac{D}{Z_0} e^{-\beta H/2}|\Psi_0\rangle\langle\Psi_0|e^{-\beta H/2}\\ &= \frac{D}{Z_0}\bigg\{ e^{-\beta H_0/2}|\Psi_0\rangle\langle\Psi_0|e^{-\beta H_0/2} - \frac{\beta}{2}\lambda e^{-\beta H_0/2}|\Psi_0\rangle\langle\Psi_0|e^{-\beta H_0/2}\int_0^1 d\xi\, e^{\beta\xi H_0/2}H_I e^{-\beta\xi H_0/2}\\ &\quad -\frac{\beta}{2}\lambda\int_0^1 d\xi\, e^{-\beta\xi H_0/2}H_I e^{\beta\xi H_0/2}e^{-\beta H_0/2}|\Psi_0\rangle\langle\Psi_0|e^{-\beta H_0/2} + \mathscr{O}(\lambda^2)\bigg\}.\end{aligned} \tag{B146}$$

In the energy basis $\{|E_{ip}\rangle = |E_i\rangle|E_p\rangle\}$ of the unperturbed system, the random wave function is given by

$$|\Psi_0\rangle = \sum_{i=1}^{D_S}\sum_{p=1}^{D_E} d_{ip}|E_{ip}\rangle, \tag{B147}$$

where d_{ip} is a Gaussian random number and $\sum_{ip}|d_{ip}|^2 = 1$. Hence, the density matrix of the random state is given by

$$|\Psi_0\rangle\langle\Psi_0| = \sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E} d_{ip}d_{jq}^*|E_{ip}\rangle\langle E_{jq}|. \tag{B148}$$

Tracing out the degrees of freedom of the environment, one has

$$\mathrm{Tr}_E|\Psi_0\rangle\langle\Psi_0| = \sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E} d_{ip}d_{jp}^*|E_i\rangle\langle E_j|. \tag{B149}$$

Substituting Eq. (B148) into Eq. (B146), the density matrix of the entirety $S+E$ reads

$$\begin{aligned}\rho &\approx \frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E} d_{ip}d_{jq}^*\bigg\{ e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_{jq}|e^{-\beta E_{jq}/2} - \frac{\beta}{2}\lambda e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_{jq}|e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}H_I e^{-\beta\xi H_0/2}\\ &\quad -\frac{\beta}{2}\lambda\int_0^1 d\xi\, e^{-\beta\xi H_0/2}H_I e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_{jq}|e^{-\beta E_{jq}/2} + \cdots\bigg\}.\end{aligned} \tag{B150}$$

Tracing out the degrees of freedom of the environment, we obtain the reduced density matrix of the system S,

$$\begin{aligned}\widetilde{\rho} = \mathrm{Tr}_E\rho &\approx \frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d_{jq}^*\bigg\{ e^{-\beta E_{ip}/2}\langle E_l|E_{ip}\rangle\langle E_{jq}|E_l\rangle e^{-\beta E_{jq}/2}\\ &\quad -\frac{\beta}{2}\lambda e^{-\beta E_{ip}/2}\langle E_l|E_{ip}\rangle\langle E_{jq}|e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}H_I e^{-\beta\xi H_0/2}|E_l\rangle\\ &\quad -\frac{\beta}{2}\langle E_l|\lambda\int_0^1 d\xi\, e^{-\beta\xi H_0/2}H_I e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_{jq}|E_l\rangle e^{-\beta E_{jq}/2} + \cdots\bigg\}\\ &= \frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d_{jq}^*\bigg\{ e^{-\beta E_{ip}/2}\delta_{lp}|E_i\rangle\langle E_j|\delta_{lq}e^{-\beta E_{jq}/2}\\ &\quad -\frac{\beta}{2}\lambda e^{-\beta E_{ip}/2}\delta_{lp}|E_i\rangle\langle E_{jq}|e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}H_I e^{-\beta\xi H_0/2}|E_l\rangle\\ &\quad -\frac{\beta}{2}\langle E_l|\lambda\int_0^1 d\xi\, e^{-\beta\xi H_0/2}H_I e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_j|\delta_{lq}e^{-\beta E_{jq}/2} + \cdots\bigg\}.\end{aligned} \tag{B151}$$

Then the elements of the reduced density matrix of the system S, in the basis that diagonalizes H_S, reads

$$\begin{aligned}\widetilde{\rho}_{i'j'} = \langle E_{i'}|\widetilde{\rho}|E_{j'}\rangle &\approx \frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d_{jq}^*\bigg\{ e^{-\beta E_{ip}/2}\delta_{lp}\langle E_{i'}|E_i\rangle\langle E_j|E_{j'}\rangle\delta_{lq}e^{-\beta E_{jq}/2}\\ &\quad -\frac{\beta}{2}\lambda e^{-\beta E_{ip}/2}\delta_{lp}\langle E_{i'}|E_i\rangle\langle E_{jq}|e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}H_I e^{-\beta\xi H_0/2}|E_l\rangle|E_{j'}\rangle\\ &\quad -\frac{\beta}{2}\lambda\langle E_{i'}|\langle E_l|\int_0^1 d\xi\, e^{-\beta\xi H_0/2}H_I e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}|E_{ip}\rangle\langle E_j|E_{j'}\rangle\delta_{lq}e^{-\beta E_{jq}/2} + \cdots\bigg\}\end{aligned}$$

$$
\begin{aligned}
&= \frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d^*_{jq}\Bigg\{ e^{-\beta E_{ip}/2}\delta_{lp}\delta_{i'i}\delta_{j'j}\delta_{lq}e^{-\beta E_{jq}/2} \\
&\quad -\frac{\beta}{2}\lambda e^{-\beta E_{ip}/2}\delta_{lp}\delta_{i'i}e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}\langle E_{jq}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2} \\
&\quad -\frac{\beta}{2}\lambda\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}\delta_{j'j}\delta_{lq}e^{-\beta E_{jq}/2} + \cdots \Bigg\}. \qquad \text{(B152)}
\end{aligned}
$$

Let us look at the different orders of terms λ of the reduced density matrix. The zero order is

$$
\mathscr{O}(\widetilde{\rho}_{i'j'})_{\lambda^0} = \frac{D}{Z_0}\sum_{l=1}^{D_E} d_{i'l}d^*_{j'l}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}, \qquad \text{(B153)}
$$

which is the term we have analyzed for the uncoupled entirety. The first order is

$$
\begin{aligned}
\mathscr{O}(\widetilde{\rho}_{i'j'})_{\lambda^1} &= -\frac{\beta}{2}\lambda\frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{j=1}^{D_S}\sum_{p=1}^{D_E}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d^*_{jq}\Bigg\{ e^{-\beta E_{ip}/2}\delta_{lp}\delta_{i'i}e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}\langle E_{jq}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2} \\
&\quad + \int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}\delta_{j'j}\delta_{lq}e^{-\beta E_{jq}/2}\Bigg\} \\
&= -\frac{\beta}{2}\lambda\frac{D}{Z_0}\sum_{j=1}^{D_S}\sum_{q=1}^{D_E}\sum_{l=1}^{D_E} d_{i'l}d^*_{jq}e^{-\beta E_{i'l}/2}e^{-\beta E_{jq}/2}\int_0^1 d\xi\, e^{\beta\xi E_{jq}/2}\langle E_{jq}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2} \\
&\quad - \frac{\beta}{2}\lambda\frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l=1}^{D_E} d_{ip}d^*_{j'l}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{ip}/2}e^{-\beta E_{j'l}/2} \\
(\boldsymbol{j\to i, q\to p}) \quad &= -\frac{\beta}{2}\lambda\frac{D}{Z_0}\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l=1}^{D_E} e^{-\beta E_{ip}/2}\Bigg\{ d_{i'l}d^*_{ip}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2} \\
&\quad + d_{ip}d^*_{j'l}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l}/2}\Bigg\}. \qquad \text{(B154)}
\end{aligned}
$$

The bold fonts inside parenthesis to the left of the equal sign are used to show and organize transformations used to go from one term to the next. We also need the complex conjugate of the reduced density matrix. The zero order is

$$
\mathscr{O}(\widetilde{\rho}^*_{i'j'})_{\lambda^0} = \frac{D}{Z_0}\sum_{l''=1}^{D_E} d^*_{i'l''}d_{j'l''}e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}. \qquad \text{(B155)}
$$

The first order is ($\langle E_{ip}|H_I|E_{jq}\rangle$ is real for the Hamiltonian we are interested in.)

$$
\begin{aligned}
\mathscr{O}(\widetilde{\rho}^*_{i'j'})_{\lambda^1} &= -\frac{\beta}{2}\lambda\frac{D}{Z_0}\sum_{i'''=1}^{D_S}\sum_{p'''=1}^{D_E}\sum_{l'''=1}^{D_E} e^{-\beta E_{i'''p'''}/2}\Bigg\{ d^*_{i'l'''}d_{i'''p'''}e^{-\beta E_{i'l'''}/2}\int_0^1 d\xi\, e^{\beta\xi E_{i'''p'''}/2}\langle E_{i'''p'''}|H_I|E_{j'l'''}\rangle e^{-\beta\xi E_{j'l'''}/2} \\
&\quad + d^*_{i'''p'''}d_{j'l'''}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l'''}/2}\langle E_{i'l'''}|H_I|E_{i'''p'''}\rangle e^{\beta\xi E_{i'''p'''}/2}e^{-\beta E_{j'l'''}/2}\Bigg\}. \qquad \text{(B156)}
\end{aligned}
$$

The expectation value for σ^2 that we want to calculate is

$$
\mathscr{E}(2\sigma^2) = \mathscr{E}\left(\sum_{i'\neq j'}|\widetilde{\rho}_{i'j'}|^2\right) = \sum_{i'\neq j'}^{D_S}\mathscr{E}(|\widetilde{\rho}_{i'j'}|^2) = \sum_{i'\neq j'}^{D_S}\mathscr{E}(\widetilde{\rho}_{i'j'}\widetilde{\rho}^*_{i'j'}). \qquad \text{(B157)}
$$

The order λ^0 term for σ^2 is

$$
\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^0} = \sum_{i'\neq j'}^{D_S}\mathscr{E}(\mathscr{O}(\widetilde{\rho}_{i'j'}\widetilde{\rho}^*_{i'j'})_{\mathscr{O}(\lambda^0)}) = \left(\frac{D}{Z_0}\right)^2\sum_{i'\neq j'}^{D_S}\sum_{l=1}^{D_E}\sum_{l''=1}^{D_E}\mathscr{E}(d_{i'l}d^*_{j'l}d^*_{i'l''}d_{j'l''})e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}, \qquad \text{(B158)}
$$

which is the term being analyzed for the uncoupled entirety with the approximation in the main text.

The order λ^1 term for σ^2 is (in the following, **a** and **b** are symbols for the calculation terms)

$$
\begin{aligned}
\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} &= \sum_{i'\neq j'}^{D_S}\mathscr{E}(\mathscr{O}(\widetilde{\rho}_{i'j'}\widetilde{\rho}^*_{i'j'})_{\lambda^1}) = \sum_{i'\neq j'}^{D_S}\mathscr{E}(\mathscr{O}(\widetilde{\rho}_{i'j'})_{\lambda^0}\mathscr{O}(\widetilde{\rho}^*_{i'j'})_{\lambda^1} + \mathscr{O}(\widetilde{\rho}_{i'j'})_{\lambda^1}\mathscr{O}(\widetilde{\rho}^*_{i'j'})_{\lambda^0})\\
&= \mathbf{ab}^* + \mathbf{a}^*\mathbf{b} = -\left(\frac{D}{Z_0}\right)^2\frac{\beta}{2}\lambda\sum_{i'\neq j'}^{D_S}\mathscr{E}\Bigg(\\
&\textbf{(Put a)} \qquad \sum_{l=1}^{D_E} d_{i'l}d^*_{j'l}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}\\
&\Big(\textbf{Put b}^*\Big|^{i'''\to i}_{p'''\to p}\Big|^{l'''\to l''}\Big) \qquad \times\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l''=1}^{D_E} e^{-\beta E_{ip}/2}\bigg\{d^*_{i'l''}d_{ip}e^{-\beta E_{i'l''}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l''}\rangle e^{-\beta\xi E_{j'l''}/2}\\
&\qquad + d^*_{ip}d_{j'l''}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l''}/2}\langle E_{i'l''}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l''}/2}\bigg\}\\
&\textbf{(Put a}^*\textbf{)} \qquad +\sum_{l''=1}^{D_E} d^*_{i'l''}d_{j'l''}e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}\\
&\textbf{(Put b)} \qquad \times\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l=1}^{D_E} e^{-\beta E_{ip}/2}\bigg\{d_{i'l}d^*_{ip}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&\qquad + d_{ip}d^*_{j'l}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l}/2}\bigg\}\Bigg).
\end{aligned}
\tag{B159}
$$

The summation indices are all the same, so we pull them out of the sum

$$
\begin{aligned}
\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} &= -\left(\frac{D}{Z_0}\right)^2\frac{\beta}{2}\lambda\sum_{i'\neq j'}^{D_S}\mathscr{E}\Bigg(\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l''=1}^{D_E}\sum_{l=1}^{D_E}\bigg[\\
&\textbf{(Put a)} \qquad d_{i'l}d^*_{j'l}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}\\
&\textbf{(Put b}^*\textbf{)} \qquad \times e^{-\beta E_{ip}/2}\bigg\{d^*_{i'l''}d_{ip}e^{-\beta E_{i'l''}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l''}\rangle e^{-\beta\xi E_{j'l''}/2}\\
&\qquad + d^*_{ip}d_{j'l''}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l''}/2}\langle E_{i'l''}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l''}/2}\bigg\}\\
&\textbf{(Put a}^*\textbf{)} \qquad + d^*_{i'l''}d_{j'l''}e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}\\
&\textbf{(Put b)} \qquad \times e^{-\beta E_{ip}/2}\bigg\{d_{i'l}d^*_{ip}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&\qquad + d_{ip}d^*_{j'l}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l}/2}\bigg\}\bigg]\Bigg).
\end{aligned}
\tag{B160}
$$

Rearranging the terms, one has

$$
\begin{aligned}
\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} &= -\left(\frac{D}{Z_0}\right)^2\frac{\beta}{2}\lambda\sum_{i'\neq j'}^{D_S}\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l''=1}^{D_E}\sum_{l=1}^{D_E}\bigg[\\
&\quad e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}\\
&\textbf{(Put ab}^*\textbf{)} \qquad \times e^{-\beta E_{ip}/2}\bigg\{\mathscr{E}(d_{i'l}d^*_{j'l}d^*_{i'l''}d_{ip})e^{-\beta E_{i'l''}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l''}\rangle e^{-\beta\xi E_{j'l''}/2}
\end{aligned}
$$

$$\begin{aligned}
&+\mathscr{E}(d_{i'l}d^*_{j'l}d^*_{ip}d_{j'l''})\int_0^1 d\xi\, e^{-\beta\xi E_{i'l''}/2}\langle E_{i'l''}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l''}/2}\Bigg\}\\
&+e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}\\
\textbf{(Put }\mathbf{a}^*\mathbf{b}\textbf{)}\qquad &\times e^{-\beta E_{ip}/2}\Bigg\{\mathscr{E}(d^*_{i'l''}d_{j'l''}d_{i'l}d^*_{ip})e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&+\mathscr{E}(d^*_{i'l''}d_{j'l''}d_{ip}d^*_{j'l})\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l}/2}\Bigg\}\Bigg].
\end{aligned}\tag{B161}$$

We want to use the expectation value identities

$$\mathscr{E}(d_\alpha d_\beta d^*_\gamma d^*_\delta)=\mathscr{E}(|d|^2|d|^2)(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})+\mathscr{E}(|d|^4)\delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta}.\tag{B162}$$

Notice that we do not have the term $\mathscr{E}(|d|^4)$ as the indices $i'\neq j'$. We check the terms $\mathscr{E}(|d|^2|d|^2)$,

$$\mathscr{E}(d_{i'l}d^*_{j'l}d^*_{i'l''}d_{ip})=\mathscr{E}(|d|^2|d|^2)\delta_{i'l,i'l''}\delta_{j'l,ip},\tag{B163}$$

$$\mathscr{E}(d_{i'l}d^*_{j'l}d^*_{ip}d_{j'l''})=\mathscr{E}(|d|^2|d|^2)\delta_{i'l,ip}\delta_{j'l,j'l''},\tag{B164}$$

$$\mathscr{E}(d^*_{i'l''}d_{j'l''}d_{i'l}d^*_{ip})=\mathscr{E}(|d|^2|d|^2)\delta_{i'l'',i'l}\delta_{j'l'',ip},\tag{B165}$$

$$\mathscr{E}(d^*_{i'l''}d_{j'l''}d_{ip}d^*_{j'l})=\mathscr{E}(|d|^2|d|^2)\delta_{i'l'',ip}\delta_{j'l'',j'l}.\tag{B166}$$

Then we have

$$\begin{aligned}
\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1}=&-\left(\frac{D}{Z_0}\right)^2\frac{\beta}{2}\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i'\neq j'}^{D_S}\sum_{i=1}^{D_S}\sum_{p=1}^{D_E}\sum_{l''=1}^{D_E}\sum_{l=1}^{D_E}\Bigg[\\
&e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}\\
\textbf{(Put }\mathbf{ab}^*\textbf{)}\qquad &\times e^{-\beta E_{ip}/2}\Bigg\{\delta_{i'l,i'l''}\delta_{j'l,ip}e^{-\beta E_{i'l''}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l''}\rangle e^{-\beta\xi E_{j'l''}/2}\\
&+\delta_{i'l,ip}\delta_{j'l,j'l''}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l''}/2}\langle E_{i'l''}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l''}/2}\Bigg\}\\
&+e^{-\beta E_{i'l''}/2}e^{-\beta E_{j'l''}/2}\\
\textbf{(Put }\mathbf{a}^*\mathbf{b}\textbf{)}\qquad &\times e^{-\beta E_{ip}/2}\Bigg\{\delta_{i'l'',i'l}\delta_{j'l'',ip}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{ip}/2}\langle E_{ip}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&+\delta_{i'l'',ip}\delta_{j'l'',j'l}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{ip}\rangle e^{\beta\xi E_{ip}/2}e^{-\beta E_{j'l}/2}\Bigg\}\Bigg]
\end{aligned}\tag{B167}$$

$$\begin{aligned}
=&-\left(\frac{D}{Z_0}\right)^2\frac{\beta}{2}\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i'\neq j'}^{D_S}\Bigg[\\
\textbf{(Put }\mathbf{ab}^*\textbf{)}\qquad &\Bigg\{\sum_{l=1}^{D_E}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{j'l}/2}\langle E_{j'l}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&+\sum_{l=1}^{D_E}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{i'l}\rangle e^{\beta\xi E_{i'l}/2}e^{-\beta E_{j'l}/2}\Bigg\}\\
\textbf{(Put }\mathbf{a}^*\mathbf{b}\textbf{)}\qquad &+\Bigg\{\sum_{l=1}^{D_E}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{\beta\xi E_{j'l}/2}\langle E_{j'l}|H_I|E_{j'l}\rangle e^{-\beta\xi E_{j'l}/2}\\
&+\sum_{l=1}^{D_E}e^{-\beta E_{i'l}/2}e^{-\beta E_{j'l}/2}e^{-\beta E_{i'l}/2}\int_0^1 d\xi\, e^{-\beta\xi E_{i'l}/2}\langle E_{i'l}|H_I|E_{i'l}\rangle e^{\beta\xi E_{i'l}/2}e^{-\beta E_{j'l}/2}\Bigg\}\Bigg]
\end{aligned}$$

$$= -\left(\frac{D}{Z_0}\right)^2 \frac{\beta}{2}\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i'\neq j'}^{D_S}\sum_{l=1}^{D_E}[$$

$$\textbf{(Put ab}^*\textbf{)}\qquad \{e^{-\beta E_{i'l}}e^{-\beta E_{j'l}}\langle E_{j'l}|H_I|E_{j'l}\rangle + e^{-\beta E_{i'l}}e^{-\beta E_{j'l}}\langle E_{i'l}|H_I|E_{i'l}\rangle\}$$

$$\textbf{(Put a}^*\textbf{b)}\qquad +\{e^{-\beta E_{i'l}}e^{-\beta E_{j'l}}\langle E_{j'l}|H_I|E_{j'l}\rangle + e^{-\beta E_{i'l}}e^{-\beta E_{j'l}}\langle E_{i'l}|H_I|E_{i'l}\rangle\}]. \tag{B168}$$

The final results for the first-order term of σ^2 is

$$\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} = -\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i'\neq j'}^{D_S}\sum_{l=1}^{D_E} e^{-\beta E_{i'l}}e^{-\beta E_{j'l}}(\langle E_{j'l}|H_I|E_{j'l}\rangle + \langle E_{i'l}|H_I|E_{i'l}\rangle). \tag{B169}$$

Changing the indices $i' \to i$, $j' \to j$, and $l \to p$, we have

$$\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} = -\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i\neq j}^{D_S}\sum_{p=1}^{D_E} e^{-\beta E_{ip}}e^{-\beta E_{jp}}(\langle E_{ip}|H_I|E_{ip}\rangle + \langle E_{jp}|H_I|E_{jp}\rangle). \tag{B170}$$

Note that if one sets $\beta = 0$, the first order is zero and the results for the X state from [39] are retrieved.

Changing the sum

$$\sum_{i\neq j}^{D_S} \Rightarrow \sum_{i}^{D_S}\sum_{j}^{D_S}(1-\delta_{ij}) \tag{B171}$$

gives

$$\begin{aligned}
&\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1}\\
&= -\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\sum_{i}^{D_S}\sum_{j}^{D_S}(1-\delta_{ij})\sum_{p=1}^{D_E} e^{-\beta E_{ip}}e^{-\beta E_{jp}}(\langle E_{ip}|H_I|E_{ip}\rangle + \langle E_{jp}|H_I|E_{jp}\rangle)\\
&= -\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\left[\sum_{i}^{D_S}\sum_{j}^{D_S}\sum_{p=1}^{D_E} e^{-\beta E_{ip}}e^{-\beta E_{jp}}(\langle E_{ip}|H_I|E_{ip}\rangle + \langle E_{jp}|H_I|E_{jp}\rangle) - 2\sum_{i}^{D_S}\sum_{p=1}^{D_E} e^{-2\beta E_{ip}}\langle E_{ip}|H_I|E_{ip}\rangle\right]\\
&= -2\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\left[\sum_{i}^{D_S}\sum_{j}^{D_S}\sum_{p=1}^{D_E} e^{-\beta E_{ip}}e^{-\beta E_{jp}}\langle E_{ip}|H_I|E_{ip}\rangle - \sum_{i}^{D_S}\sum_{p=1}^{D_E} e^{-2\beta E_{ip}}\langle E_{ip}|H_I|E_{ip}\rangle\right]\\
&= -2\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\left[\sum_{i}^{D_S}\sum_{j}^{D_S}\sum_{p=1}^{D_E} e^{-\beta E_{i}}e^{-\beta E_{j}}e^{-2\beta E_p}\langle E_{ip}|H_I|E_{ip}\rangle - \sum_{i}^{D_S}\sum_{p=1}^{D_E} e^{-2\beta E_{ip}}\langle E_{ip}|H_I|E_{ip}\rangle\right]\\
&= -2\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)\left[\sum_{j}^{D_S} e^{-\beta E_j}\sum_{i}^{D_S}\sum_{p=1}^{D_E} e^{-\beta E_{i}}e^{-2\beta E_p}\langle E_{ip}|H_I|E_{ip}\rangle - \sum_{i}^{D_S}\sum_{p=1}^{D_E} e^{-2\beta E_{ip}}\langle E_{ip}|H_I|E_{ip}\rangle\right]\\
&= -2\left(\frac{D}{Z_0}\right)^2 \beta\lambda\mathscr{E}(|d|^2|d|^2)[Z_S\mathrm{Tr}e^{-\beta H_S}e^{-2\beta H_E}H_I - \mathrm{Tr}e^{-2\beta(H_S+H_E)}H_I].
\end{aligned} \tag{B172}$$

By applying the same symmetry argument as above, transform $S \to -S$ and $I \to I$ or, alternatively, transform $S \to S$ and $I \to -I$, one has

$$\mathrm{Tr}e^{-\beta H_S}e^{-2\beta H_E}H_I = \mathrm{Tr}e^{-\beta H_S}e^{-2\beta H_E}U^+H_IU = -\mathrm{Tr}e^{-\beta H_S}e^{-2\beta H_E}H_I, \tag{B173}$$

$$\mathrm{Tr}e^{-2\beta(H_S+H_E)}H_I = \mathrm{Tr}e^{-2\beta(H_S+H_E)}U^+H_IU = -\mathrm{Tr}e^{-2\beta(H_S+H_E)}H_I. \tag{B174}$$

The terms of traces have to be zero. Therefore, if there exists such symmetry in the entirety $S + E$, such as the system with the Hamiltonian described in Eqs. (B139)–(B141), the first order of σ^2 is

$$\mathscr{O}(\mathscr{E}(2\sigma^2))_{\lambda^1} = 0. \tag{B175}$$

Calculating the second-order term of σ^2 is much more complicated as the perturbation term comes from both the denominator and numerator of Eq. (B6). We are not going to calculate the second-order term of σ^2. We may conjecture that the second-order term is zero from the simulation results, and the σ of the uncoupled entirety is a lower bond for the σ of the coupled entirety.

We have not calculated the first-order term for $\mathscr{E}(\delta^2)$. However, the numerical results from Appendix A can be used to form an ansatz that the first-order term either vanishes or is small for Hamiltonians with the symmetry that makes the first-order term of $\mathscr{E}(\sigma^2)$ be zero.

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