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Quantum criticality at high temperature revealed by spin echo

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Abstract. Quantum criticality occurs when the ground state of a macroscopic quantum system changes abruptly on tuning system parameters. It is an important indicator of new quantum matters emerging. In conventional methods, quantum criticality is observable only at zero or low temperature (as compared with the interaction strength in the system). We find that a quantum probe, if its coherence time is long, can detect the quantum criticality of a system at high temperature. In particular, the echo control over a spin probe can remove the thermal fluctuation effects and hence reveal the critical quantum fluctuation without requiring low temperature. We first use the exact solution of the one-dimensional transverse-field Ising model to demonstrate the possibility of detecting the quantum criticality at high temperature by spin echo. The critical behaviors were calculated using the exact solution and understood by the noise spectrum analysis in the Gaussian noise approximation. By numerical simulation, we further verify that the high-temperature quantum criticality also exists in the probe coherence measurement of spin systems with dipolar couplings. Using the noise spectrum analysis, we establish the correspondence between the necessary low temperature ($T_{QC}$) in conventional methods and the necessary long coherence time ($t_{QC}$) in probe decoherence measurement to observe the quantum criticality, that is, $T_{QC} \sim 1/t_{QC}$ and much less than the interaction strength of the system. For example, probes with quantum coherence times of milliseconds or seconds can be used to study, without cooling the

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Quantum phase transitions [1] occur when the ground states of macroscopic quantum systems change abruptly on tuning system parameters (such as external fields or internal interaction strengths). Quantum criticality accompanies quantum phase transitions as a result of the critical behaviors of quantum fluctuations. Quantum criticality is important as it signifies the emergence of new quantum matters and new physics [2–10]. The critical quantum fluctuations also exist at non-zero temperatures. However, at a temperature higher than the system’s interaction strength (Planck and Boltzmann constants taken as unity hereafter), thermal fluctuations will conceal the quantum criticality. Extremely low temperatures are required for quantum criticality to be observed in many interesting systems by conventional methods (e.g. magnetic susceptibility measurement). For example, for nuclear spins in solids [5–7] and cold atoms in optical lattices [8–10], temperatures of $10^{-9}$ or even $10^{-12}$ K are required [7, 11]. Such a limitation excludes many new classes of quantum matters and hence new physics from experimental investigation.

In this paper, we show that quantum criticality can be observed at temperatures much higher than the interaction strength by measuring the echo signal of a probe spin coupled to a quantum many-body system, because the spin echo can remove the thermal fluctuation effect [12] and therefore reveal the quantum fluctuation effect. We discover the correspondence between the low temperature ($T_{QC}$) required in conventional methods and the long coherence time ($t_{QC}$) required in probe decoherence measurement to observe the quantum criticality, that is, $T_{QC} \sim 1/t_{QC}$ and much less than the interaction strength of the system. For example, quantum criticality that would require temperatures as low as $10^{-9}$ or even $10^{-12}$ K to be observed in conventional methods can be detected at high temperature by a probe spin with coherence times...
longer than milliseconds or seconds, respectively. Such long coherence times have already been realized in a wide range of realistic physical systems [13–16]. For example, nitrogen–vacancy (NV) centers can be implanted beneath the diamond surface [14] as a probe to study the dynamics of the spins placed on the surface. The spin echo probe method provides a possibility to study the quantum criticality of a system without cooling the system to an extremely low temperature (which is required in conventional susceptibility measurement).

The key is to devise a time-dependent measurement sensitive to the quantum fluctuations but immune to thermal noises. A previous study proposed that quantum criticality can be probed by the Loschmidt echo [17], which is equivalent to free-induction decay (FID) of a probe spin. The critical features of the long-time behaviors of the Loschmidt echo (see e.g. [18]) are closely related to the ground state fidelity, which has been widely used to study quantum phase transitions [19, 20]. Nuclear magnetic resonance experiments that employ pseudo-pure states to simulate effective zero temperature have shown such an enhancement of FID for a three-nucleus system [21]. The Loschmidt echo or FID, however, like other conventional measurements of quantum criticality, requires that the temperature be much lower than the interaction strength of the system. In magnetic resonance spectroscopy, the spin echo can be used to eliminate the effect of thermal fluctuations (or inhomogeneous broadening) [12] with the decay of the echo signal induced mostly by quantum fluctuations. Recent studies of central spin decoherence in nanoscale spin baths revealed that when the spin echo control is applied to the central spin, quantum fluctuations are still important even at temperatures much higher than the interaction strength in the baths [22–26]. For example, an anomalous decoherence effect due to quantum fluctuations has been revealed by removing the thermal noise effect [25, 26]. Thus, we are motivated to use spin echo to study quantum criticality at high temperature.

The method proposed in this paper, particularly if applied to study quantum orders of nuclear spins, is different from the previous dynamical polarization method that produces a low effective temperature for the relatively isolated nuclear spins [5–7, 27]. Also, the present method is different from the magnetic resonance spectroscopy technique that has been widely used to study phase transitions in solids (see e.g. [28, 29]), in that the conventional methods study phase transitions that actually occur but the present method reveals quantum critical points that are not supposed to occur under the given conditions (high temperatures). We would also like to point out that quantum criticality at high temperature discussed in this paper is fundamentally different from that studied in the previous nuclear magnetic resonance experiments at room temperature [21] where the pseudo-pure states of spin ensembles were employed to simulate an effective zero temperature [30]. The pseudo-pure state method cannot be scaled up to the thermodynamic limit since the required sample size increases exponentially with the number of spins [30]. The approach in this paper involves the physical temperature (in contrast to the simulated one) and does not have the ensemble scaling issue.

2. Decoherence of a probe spin coupled to a quantum spin system

We consider the echo signal of a probe spin-1/2 coupled to a quantum spin system (a bath). To have conclusive results, we choose an exactly solvable model [1], namely, the one-dimensional Ising model in a transverse field with Hamiltonian (see appendix A)

$$H_h = -\sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \lambda \sum_{j=1}^{N} \sigma_j^z \equiv H_0 + \lambda H_1$$

(1)
with periodic boundary condition, where \( \sigma^x/\tau \) is the Pauli matrix of the \( j \)th spin along the \( x/y/z \)-axis. The probe–bath interaction is \( g \sigma^z \otimes H_1 \equiv \sigma^z \otimes B/2 \). The probe spin can be considered to be placed at the center of a ring of Ising spins. The probe strength is chosen to scale with the bath size as \( g \sim 1/\sqrt{N} \), which is \( \ll 1 \) for a large bath so that the bath is only weakly perturbed by the probe (see appendix C for a discussion about the weak probe condition). The bath at thermal equilibrium with inverse temperature \( \beta \) is described by a density matrix \( \rho = \exp(-\beta H_2) / \text{Tr}(\exp(-\beta H_2)) \). The FID of the probe spin is \( L_{\text{FID}}(t) = |\text{Tr}(e^{-iH_2 t/2} e^{iH_1 t} \rho e^{iH_2 t})| \) (see equation (A.1) in appendix A). In spin echo, the probe spin is flipped (\( \uparrow \leftrightarrow \downarrow \)) at a time \( t/2 \), and the spin coherence is measured at \( t \). The echo signal is \( L_{\text{SE}}(t) = |\text{Tr}(e^{-iH_2 t/2} e^{iH_1 t} \rho e^{iH_2 t/2} e^{iH_2 t})| \) (see equation (A.12) in appendix A). The spin chain model has no phase transition at finite temperature but has a quantum criticality between a ferromagnetic order for \( \lambda < 1 \) and a paramagnetic order for \( \lambda > 1 \) [1]. This model has been used previously to demonstrate the effect of quantum criticality on FID [17]. A previous study on spin echo for this model [31], however, missed the quantum criticality features at high temperature due to inadequate approximation. Figure 1(a) shows that the FID of the probe spin is greatly enhanced at the quantum critical point when the temperature is zero (\( \beta = \infty \)), which is consistent with a previous study [17]. The sharp dip at the critical point, however, is blurred with increasing temperature (figure B.2 in appendix B) and disappears at infinite temperature (figure 1(b)). In contrast, the spin echo signal (figure 1(c)) presents enhanced decoherence at the critical point even at infinite temperature (\( \beta = 0 \)). Both in FID and spin echo, the critical feature is pronounced only when \( t \gg 1 \).

The above-mentioned phenomena can be understood from the noise spectrum of the bath. The fluctuation of the local field \( B \equiv 2gH_1 \) has both thermal and quantum components, with the correlation function \( C(t) = \langle B(t) \rangle - \langle B(t) \rangle \langle B(0) \rangle \), where \( \langle O \rangle \equiv \text{Tr} \{ \rho O \} \) and \( \dot{O}(t) \equiv e^{iH_1 t} O e^{-iH_1 t} \). The probe spin decoherence is determined by the noise spectrum \( S(\omega) = \int C(t) \exp(\text{iot}) \, dt \) (see appendix B). The thermal fluctuation part \( S_{\text{th}}(\omega) = 2\pi \delta (\omega) \left( \sum_n P_n(\eta, \lambda) |B(\eta, \lambda)\rangle^2 - \langle B \rangle^2 \right) \equiv 2\pi \delta (\omega) C(0) \) is due to the fact that at finite temperature the bath has a probability distribution \( P_n \) in different eigenstates \( |n, \lambda \rangle \) that yield different local fields\(^3\). At zero temperature the thermal fluctuation vanishes. In general, the local field operator \( H_1 \) does not commute with the bath interaction Hamiltonian \( H_0 \). Thus transitions between different eigenstates by elementary excitations lead to quantum fluctuation. The quantum fluctuation is dynamical and has a spectrum \( S_Q(\omega) = 2\pi \sum_{n \neq m} \delta (\omega - E_n + E_m) P_n \langle |n, \lambda \rangle |m, \lambda \rangle |^2 \). At high temperature, the thermal fluctuation is usually much stronger than the quantum fluctuation. As the thermal fluctuation is static (\( S_{\text{th}}(\omega) \) is non-zero only at zero-frequency), its effect on the probe spin decoherence can be removed by spin echo [12]. Then the decoherence is determined by the dynamical quantum fluctuation. In the long-time limit, the decoherence would be mostly due to the low-frequency noise caused by low-energy or long-wavelength excitations in the bath, which are particularly important in quantum criticality. The excitation energy as a function of the wavevector is \( \varepsilon(k) = 2\sqrt{1 - 2\lambda \cos k + \lambda^2} \) (see appendix A). The excitation has a finite energy gap except for the critical point.

\(^2\) Here ‘infinite temperature’ actually means that the temperature is much higher than any other energy scales in the system. In realistic experiments, the temperature must be finite and is bounded by the validity of the Hamiltonian (which is usually the low-energy effective theory) that describes the system.

\(^3\) In principle, the thermal distribution and hence the thermal noise are due to quantum entanglement between the bath and the greater environment (the rest of the universe). Such noise fluctuates at a much longer timescale than the timescale of the probe spin decoherence and is therefore treated as ‘static’.
Figure 1. Quantum criticality in a spin chain detected by decoherence of a probe spin. (a) FID of the probe spin versus time and the external field strength $\lambda$ for the bath at zero temperature. (b) The same as (a) but for the bath at infinite temperature. (c) Echo signal of the probe spin versus time and the external field strength for the bath at infinite temperature. (d) Dispersion of elementary excitations in the bath for various external field strengths. (e) Noise spectra of quantum fluctuations at various temperatures (indicated by the inverse temperature $\beta$) for external field $\lambda = 1$. (f) The same as (e) but with $\lambda = 0.75$. The number of spins in the bath is $N = 10000$ and the probe–bath coupling $g = N^{-1/2} = 0.01$.

$\lambda = 1$ (figure 1(d)). The quantum fluctuation spectrum is gapless at the critical point (figure 1(e)) and has a low-frequency cut-off for $\lambda \neq 1$ (figure 1(f)). Gapless fluctuation emerging at the critical point is responsible for the decoherence enhancement in the long-time limit.

3. Time-inverse temperature correspondence

We further explore the correspondence between the long coherence time and the low temperature required for the quantum criticality to be observed in the spin decoherence probe and in conventional susceptibility measurement, respectively.

Figure 1(c) shows that the decoherence enhancement at the critical point is visible only at large $t$. Figure 2(a) presents the magnetic susceptibility (see equation (B.6) in appendix B) of the spin chain versus the inverse temperature $\beta$ and the external field strength $\lambda$ in the thermodynamic limit ($N \to \infty$). The quantum criticality feature is visible for large $\beta$ (e.g. $\beta > 10$), resembling the echo signal as a function of time and field strength in figure 1(c). Figure 2(b) shows clearly that the sharp features at the critical point are pronounced at similar values of $\beta$ and $t$ in the susceptibility and probe spin coherence echo, respectively.
Figure 2. Correspondence between time and inverse temperature required for quantum criticality to emerge. (a) Susceptibility of the spin chain bath as a function of the external field $\lambda$ and inverse temperature $\beta$. (b) Susceptibility of the bath (upper panel) and probe spin echo signals (lower panel) as functions of the external field $\lambda$ for various inverse temperatures $\beta$ and echo times $t$, respectively. (c) FID of the probe spin as a function of the external field for various times $t$. The coherence at $t = 20$ is amplified by $10^{120}$.

Actually, if the measurement time is long enough, even the FID would display a sudden transition at the critical point (figure 2(c)), which, however, is far beyond feasible measurement since the remaining coherence in FID is as little as $10^{-180}$ (at $t = 20$).

The probe spin decoherence and the bath susceptibility are intrinsically related to each other as both of them are caused by the local field fluctuations. Under the weak-probe condition, the probe spin decoherence is determined by the noise correlation function $C(t_1 - t_2)$ as (see appendix B)

$$\ln[L_\alpha(t)] = -\frac{1}{2} \int_0^t \int_0^{t'} dt_1 dt_2 C(t_1 - t_2) f_\alpha(t_1) f_\alpha(t_2)$$

with $\alpha = \text{FID}$ or $\text{SE}$ corresponding to the FID and the spin echo signal, respectively. The modulation functions $f_{\text{FID}}(t') = 1$ and $f_{\text{SE}}(t') = 1$ for $t' \in [0, t/2]$ and $f_{\text{SE}}(t') = -1$ for $t' \in [t/2, t]$. The magnetic susceptibility is determined by the correlation function as

$$\chi = \frac{1}{4Ng^2} \int_0^\beta d\tau C(i\tau).$$

The susceptibility has the form of the noise correlation function integrated along the imaginary axis in the complex plane of the time. Therefore for the quantum criticality to be pronounced,
the inverse temperature \(1/T_{QC}\) required in susceptibility measurement is similar to the time duration \(t_{QC}\) required in probe coherence measurement, i.e.

\[
T_{QC} \sim 1/t_{QC}
\]  

(4)

both of which should be much less than the interaction strength in the bath. A probe with long coherence time can detect, even at high temperature, quantum criticality that would be observable only at extremely low temperatures in the conventional magnetic susceptibility measurement.

4. Critical exponents

Now we study the critical behaviors at the critical point.

By Fourier transform of equation (2), the probe spin decoherence is determined by the noise spectrum as [32]

\[
\ln [L_{FID}(t)] = -C(0)t^2 - t \int_0^\infty \frac{dx}{2\pi} S_Q(x/t) M_{FID}(x),
\]

(5a)

\[
\ln [L_{SE}(t)] = -t \int_0^\infty \frac{dx}{2\pi} S_Q(x/t) M_{SE}(x),
\]

(5b)

where the filter functions \(M_{FID}(x) = \sin^2(x/2)\) and \(M_{SE}(x) = \frac{1}{16} x^2 \sin^4(x/4)\) are determined by the Fourier transform of the modulation functions \(f_{FID}(t)\) and \(f_{SE}(t)\), respectively (see equation (B.5) in appendix B). Similarly, the magnetic susceptibility of the bath is

\[
\chi(\beta) = \frac{\beta}{2} C(0) + \int_0^\infty \frac{dx}{2\pi} S_Q(x/\beta) M_{\chi}(x) \frac{dx}{2\pi}
\]

(6)

with \(M_\chi(x) = x^{-1} \tanh(x/2)\) being the corresponding filter function derived by the Fourier transform of equation (3) (also see equation (B.9) in appendix B). Above the frequency has been scaled by \(x = \omega t\) or \(\omega \beta\). The modulation functions are plotted in figures 3(a)–(c).

The probe spin FID at the critical point goes to zero as an exponential function of the evolution time at zero temperature (\(\beta = \infty\)) (figure 3(d)). In the long-time limit \((t \gg 1)\), the probe spin decoherence is determined by the low-frequency noise, so in equation (5) the quantum noise spectrum can be approximated as a constant \(S_Q(0)\). Also at zero temperature, the thermal noise is zero. Therefore, the FID at the critical point scales with time by \(\ln |L_{FID}| \approx -t S_Q(0) \int_0^\infty \frac{dx}{2\pi} M_{FID}(x) = -\frac{1}{2} t S_Q(0)\), as observed in figure 3(d). The spin echo at infinite temperature (\(\beta = 0\)) has similar scaling with time at the critical point. The filter function of spin echo (see figure 3(b)) is zero at zero frequency and has its maximum at \(\omega_0 \approx 4.7 t^{-1}\). Similar to the FID case, the low-frequency noise dominates the spin echo decay and leads to the critical scaling \(\ln |L_{SE}| \sim -\frac{1}{2} t S_Q(0)\), which is confirmed in figure 3(e). In the case of magnetic susceptibility, the modulation function approaches \(1/x\) as \(x = \omega \beta \to \infty\). As the noise spectrum has a high-frequency cut-off (see figure 1(e)), the integration in equation (6) leads to the logarithm divergence with the inverse temperature, i.e. \(\chi \sim \int e^{[\lambda+\lambda_c]\frac{1}{\beta}} x^{-1} dx \sim \ln \beta\), as observed in figure 3(f).

Figure 4 shows the respective scaling of the probe spin coherence or the susceptibility with the external field approaching the critical point \((\lambda - \lambda_c \to 0)\) for large evolution time or
Figure 3. Time scaling of the probe spin decoherence and temperature scaling of the magnetic susceptibility at the critical point. Panels (a)–(c) show in turn the filter functions for FID, spin echo and magnetic susceptibility as functions of the scaled frequency ($x = \omega t$ or $\omega \beta$). (d) The symbols are $\text{ln}|L_{\text{FID}}|$ as a function of time at $\lambda = 1$ and the solid line is the linear fitting. (e) The same as (d) but for the spin echo signal. (f) The symbols are the magnetic susceptibility as a function of $\log(\beta)$ at $\lambda = 1$ and the line is the linear fitting.

low temperature. To deduce the critical behavior at zero temperature or infinite time ($\beta, t = \infty$), we choose the temperature or time such that $|\lambda - \lambda_c| \beta / t \gg 1$ or $|\lambda - \lambda_c| \beta \gg 1$. For a large time, the scaled noise spectrum $S_Q(x/t)$ is spanned in the range from the low-frequency cut-off $4|\lambda - \lambda_c| t$ to the high-frequency cut-off $4|\lambda + \lambda_c| t$. With the condition $|\lambda - \lambda_c| t \gg 1$, the filter functions for FID or spin echo decay with the scaled frequency as $x^{-2}$. Therefore the probe spin decoherence in FID or spin echo, up to a structure factor in the order of one, $-\text{ln}|L_{\text{FID/SE}}| \sim \int_{4|\lambda - \lambda_c| t}^{4|\lambda + \lambda_c| t} x^{-2} \, dx \sim |\lambda - \lambda_c|^{-1}$, with an inverse linear divergence. Note that the divergence is determined by the low-frequency cut-off due to the excitation gap in the bath. Such a critical divergence is shown in figures 4(a)–(d). The oscillation features in the decoherence are due to the oscillations in the filter functions (see figures 3(a) and (b)). The inverse linear scaling is violated when the long-time condition $|\lambda - \lambda_c| t \gg 1$ is not fulfilled (since the filter functions converge to a constant rather than diverge as $x^{-2}$ at the zero frequency). The critical scaling of the susceptibility can be analyzed similarly. Now that the modulation function decays with frequency as $1/x$, the scaling relation becomes $\chi \sim \int_{4|\lambda - \lambda_c| t}^{4|\lambda + \lambda_c| t} x^{-1} \, dx \sim \text{ln}|\lambda - \lambda_c|$, with a logarithmic divergence, as shown in figures 4(e) and (f).

As demonstrated in figures 3 and 4, the probe coherence is actually more sensitive to the criticality than the conventional susceptibility (linear versus logarithmic divergence). This is due to the fact that the filter functions for the FID and spin echo decay faster on increasing the frequency and therefore are more sensitive to the low-frequency dynamics, which is responsible for the critical phenomena.
5. Dipolar spin-ring model

The study above on the exactly solvable transverse-field Ising model establishes rigorous evidence for the existence of quantum criticality at high temperature. It is of interest to examine whether and how such a phenomenon would present in other systems. A particularly interesting model is spins with dipolar coupling, which is often the case for interactions between real electron or nuclear spins in solids. In this section, we study the decoherence of a probe spin due to coupling to a ring of spins with dipolar coupling.

The model system is illustrated in figure 5(a). The bath spins are 20 electron spins on a ring of radius 15 nm. The probe is an electron spin 5 nm below the center of the ring. A weak magnetic field $B$ is applied along the $z$-axis (normal to the ring) to tune the bath across the critical point. The dipolar interaction between the spins depends inverse cubically on distance and the distance between bath spins is much less than the probe–bath distance, so the weak probe condition is satisfied (see appendix C for a discussion of the weak probe condition).

As shown in appendix E, the spin-ring model resembles the Heisenberg–Ising (XXZ) model.
Figure 5. Quantum criticality of a dipolar spin-ring model at high temperature. 
(a) Schematic representation of the model made of a ring of spins with a probe spin below the center of the ring. A magnetic field $B$ is applied along the $z$-axis. (b) The 20 lowest energy levels of the spin ring as functions of the external magnetic field. The inset zooms in the levels near the critical point (about 0.22 G). (c) Field dependence of the long-range correlation between two bath spins at the two ends of a diameter, $\langle S_1 \cdot n_{1/2} S_{N/2} + n_{N/2} \rangle$ with $n_j$ denoting the direction tangential to the ring at the position of the $j$th spin. The correlation is plotted for various temperatures $T = 7.6 \times 10^{-12}, 6.4 \times 10^{-6}, 8.5 \times 10^{-6}$ and $1.3 \times 10^{-5}$ K corresponding to the inverse temperatures $\beta = 1 \times 10^6, 1.2, 0.9$ and 0.6 $\mu$s in turn. Panels (d) and (e) present the FID of the probe spin at zero and infinite temperature, respectively. (f) Spin echo of the probe spin at infinite temperature. In calculation for (b)–(f), the ring contains 20 equally separated spins and has radius 15 nm, and the probe center is 5 nm below the center of the ring.

(see equation (E.3)) which has a quantum phase transition between the ferromagnetic and paramagnetic orders [33]. The details of the model and a possible physical realization are discussed in appendix E.

We numerically simulate the dipolar spin-ring system (see appendix E). To simplify the simulation, we adopted the nearest-neighbor coupling approximation for interaction between
bath spins (see justification in appendix E). As shown in figure 5(b), the ring of 20 coupled bath spins (with the coupling to the probe spin dropped) has two nearly degenerate ground states for a magnetic field below the critical value \(B_c \approx 0.22 \text{ G}\), corresponding to spontaneous ferromagnetic ordering with the spins aligned along the ring in parallel. For a field above the critical value, the ground state degeneracy is lifted and the bath is in a paramagnetic phase with the spins polarized along the magnetic field. This can be, indeed, seen from the ‘long-range’ correlations of the spins (figure 5(c)), which presents a sharp decrease near the critical point at zero temperature. The transition region has finite width as the probe–bath coupling is finite (see appendix C). As temperature increases to above \(10^{-6} \text{ K}\), however, the transition is smeared out and eventually disappears as temperature approaches the interaction strength \(\sim 2.3 \times 10^{-5} \text{ K or } 3.1 \mu s^{-1}\) between neighboring bath spins.

The FID of the probe spin at zero temperature is enhanced near the critical point (figure 5(d)). The decoherence, however, is far from complete and presents oscillation features, which is a finite-size effect (the oscillation period near the critical point is proportional to the number of spins in the ring). As temperature increases, the thermal fluctuation and hence the decoherence are enhanced, so the transition near the critical point is smeared out. At infinite temperature, the decoherence presents no critical feature except that a periodic revival structure appears in the paramagnetic phase but is absent in the ferromagnetic phase (figure 5(e)). Such revival, however, is an effect of finite and uniform probe strength (see appendix D and figure D.1). While the revivals of FID signals provide an interesting detection of quantum criticality in finite systems at high temperature, the strong thermal fluctuation in general macroscopic systems would, however, conceal the quantum criticality.

The spin echo signal (figure 5(f)) shows a sudden change at the critical point even at infinite temperature. Unlike the Ising model studied in figures 1 and 2, the dipolar spin model presents a step feature rather than a dip in the spin echo decay. This can be understood as follows. In the dipolar spin model, there are spin interactions in all directions, so strong low-frequency quantum fluctuation along the \(z\)-direction exists in the ferromagnetic phase. In contrast, in the transverse-field Ising model which has unidirectional interaction between the spins, the quantum fluctuation along the \(z\)-axis would be strongly suppressed in the ferromagnetic phase. In the paramagnetic phase (for both the Ising model and the dipolar spin model), the spins are polarized along the field direction (the \(z\)-axis); the quantum fluctuation along the \(z\)-axis therefore has an energy gap, i.e. the low-frequency fluctuation is suppressed.

6. Perspectives for experimental observation

A broad range of physical systems may be considered for studying quantum criticality at high temperature. Such systems should satisfy the following conditions. Firstly, there is a parameter such as an external field that is tunable across a quantum critical point; secondly, there exists a quantum probe with coherence time that can be extended (by spin echo, e.g.) to be much longer than the inverse interaction strength in the bath; and thirdly, the probe–bath interaction is much weaker than the intra-bath interaction so that the bath dynamics is not strongly perturbed (otherwise the transition region would be broad, as shown in appendix C figure C.1).

Among numerous possible systems, a few examples are cold atoms in optical lattices or traps, defect spins in diamond, donor spins in silicon and nuclear spins in large molecules. The
probe spins in such systems have long coherence times that range from milliseconds to nearly 10 s [13–16]. It is still a non-trivial technical challenge to assemble a large number of spins in regular configurations that resemble the quantum spin models such as those studied in this paper. However, with the rapid advances in precise positioning, controlling and detecting single spins in solids [34–39] and single ions in traps [40, 41], it is not inconceivable to realize the spin echo probe of the quantum magnetism models. In particular, phosphorous impurities may be implanted in silicon with atomic precision [34–37] and the electron or nuclear spins of the P impurities can form a dipolar spin system as studied in section 5. Such a dipolar system may also be realized by coupling a NV center spin near a diamond surface to a ring of electron spins placed on the surface [38, 39]. Interactions between spins of trapped ions can be engineered to such an extent [40, 41] that various quantum spin models including the Ising model and the XXZ model can be realized. Cold atoms in spin-dependent optical lattices [42] will also be promising candidate systems with the internal spins acting as the probe.

It is noteworthy that although the study in this paper assumes a single spin probe, it is straightforward to generalize the method to an ensemble of probe spins without mutual interactions. Generalization to correlated probe spin ensembles is also possible but further study is still needed.

7. Conclusion

In summary, we propose a new approach to study quantum criticality, in lieu of lowering temperature to the critical regime. The time-inverse temperature correspondence enables utilization of long coherence time to detect at high temperature quantum criticality and hence new quantum matters which would occur at extremely low temperature. The exact solution of the transverse-field Ising model provides rigorous evidence for existence of the phenomenon. The numerical solution of a dipolar spin-ring model indicates that the phenomenon may also exist in other quantum spin systems. Further study, however, is needed to classify how different systems would present the quantum criticality at high temperature. It is also of interest to examine models that have finite-temperature phase transitions.

A wide range of quantum probes have coherence time from milliseconds to seconds [13–16], and therefore can be used to study physics that would otherwise emerge at nano-kelvin to pico-kelvin. Spin echo, by largely removing the thermal fluctuation effect, can prolong the coherence time of a quantum probe. It is conceivable that longer coherence time and therefore richer physics can be brought into the reach by applying many-pulse dynamical decoupling control over the probe [24, 43–45]. Therefore, it is envisaged that dynamical decoupling will become a useful tool to study many-body correlations in baths, beyond its existing applications in noise spectrum measurement [46] and high-sensitivity metrology [47].

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Appendix A. Exact solution of the transverse-field Ising model

The Hamiltonian in equation (1) is block diagonalized and can be written as $H = H_{z+g} \otimes |\uparrow\rangle \langle \uparrow| + H_{z-g} \otimes |\downarrow\rangle \langle \downarrow|$, by which the spin bath is driven by different Hamiltonians depending on the probe spin state $|\uparrow/\downarrow\rangle$. We prepare the probe spin on a coherent state $|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle) / \sqrt{2}$. If the bath is initially in a thermal equilibrium state $\rho$, the coherence of the probe spin is

$$L_{\text{FID}} = \left| \text{Tr} \left[ |\uparrow\rangle \langle \uparrow| e^{-iHt} \rho \otimes |\psi\rangle \langle \psi| e^{iHt} \right] \right| = \left| \text{Tr}(e^{-iH_{z+g}t} \rho e^{iH_{z-g}t}) \right|.$$ \hspace{1cm} (A.1)

The one-dimensional transverse-field Ising model can be solved exactly [1]. By applying Jordan–Wigner transformation [1]

$$\sigma_j^x = 1 - 2a_j^\dagger a_j, \quad \sigma_j^y + i\sigma_j^z = 2\left( \prod_{i<j} \sigma_i^z \right) a_j$$ \hspace{1cm} (A.2)

the Hamiltonian is transformed to be a free-fermion one as

$$H_s = - \sum_{j=1}^{N} [(a_j^\dagger - a_j)(a_{j+1}^\dagger + a_{j+1}) - 2\lambda a_j^\dagger a_j] - N\lambda,$$ \hspace{1cm} (A.3)

where $a_j$ and $a_j^\dagger$ are the annihilation and creation fermion operators at the $j$th site, respectively. Here, we choose the boundary condition according to the parity ($P = \prod_{j=1}^{N} \sigma_j^z$) of the system, namely, $c_{N+1} = \pm c_1$ for $P = \pm 1$. By Fourier transform $a_j = \sum_k c_k \exp(-ikj) \sqrt{N}$, the spin system is mapped to a spinless fermion system

$$H_k = - \sum_k [(2\cos k - 2\lambda) c_k^\dagger c_k + i \sin k (c_{-k}^\dagger c_k^\dagger + c_{-k} c_k)] - N\lambda,$$ \hspace{1cm} (A.4)

where $c_k^\dagger$ and $c_k$ are creation and annihilation operators of fermions with wavevector $k$, respectively. The vacuum state of the modes with momenta $k$ and $-k$ is $|0_{-k}, 0_k\rangle$. This Hamiltonian can be diagonalized by the Bogoliubov transformation [1]

$$\begin{pmatrix} b_{-k} \\ b_k^\dagger \\ b_{-k}^\dagger \\ b_k \end{pmatrix} = \begin{pmatrix} u_k & 0 & 0 & iv_k \\ 0 & u_k & -iv_k & 0 \\ 0 & -iv_k & u_k & 0 \\ iv_k & 0 & 0 & u_k \end{pmatrix} \begin{pmatrix} c_{-k} \\ c_k \\ c_{-k}^\dagger \\ c_k^\dagger \end{pmatrix},$$ \hspace{1cm} (A.5)

where $u_k = \cos \theta_k$, $v_k = \sin \theta_k$ with $\tan(2\theta_k) = \sin k / (\cos k - \lambda)$. After the transform, the diagonalized fermion Hamiltonian

$$H_k = \sum_k \varepsilon_k (b_k^\dagger b_k - 1/2)$$ \hspace{1cm} (A.6)

with dispersion

$$\varepsilon_k = 2\sqrt{1 - 2\lambda \cos k + \lambda^2}.$$ \hspace{1cm} (A.7)

The transformed vacuum state of the modes with momenta $k$ and $-k$ is $|0_{-k}, 0_k\rangle$. The ground state of the Ising chain is $\otimes_{k>0} |0_{-k}, 0_k\rangle$ since all quasi-particles have positive energy.
The excited states are obtained by applying the creation operators $b_k^\dagger$ to the ground state. The transform between the Fock states corresponding to different sets of fermion operators is

$$
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|0_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix} =
\begin{pmatrix}
u_k & 0 & 0 & 0 \\
0 & u_k & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|1_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix}.
$$ (A.8)

The coherence of the center spin in the case of FID is

$$
L_{\text{FID}}(t) = \prod_{k > 0} \text{Tr}[\rho_k U_{k,+}(t)U_{k,-}(t)]
$$ (A.9)

with $\rho_k$ being the $k$th component density matrix of the initial bath state

$$
\rho_k = \frac{1}{1 + 2 e^{-\beta \varepsilon_k} + e^{-2\beta \varepsilon_k}}
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|0_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix}^T
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & e^{-2\beta \varepsilon_k} & 0 & 0 \\
0 & 0 & e^{-\beta \varepsilon_k} & 0 \\
0 & 0 & 0 & e^{-\beta \varepsilon_k}
\end{pmatrix}
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|0_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix}
$$ (A.10)

and the evolution operator

$$
U_{k,\pm}(t) =
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|0_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix}^T
\begin{pmatrix}
A_\pm & -B_\pm & 0 & 0 \\
B_\pm & A_\pm^* & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
|0_{-k}, 0_k\rangle \\
|1_{-k}, 1_k\rangle \\
|0_{-k}, 1_k\rangle \\
|1_{-k}, 0_k\rangle
\end{pmatrix},
$$ (A.11)

where $A_\pm \equiv \cos(\varepsilon_{k,\pm} t) + i \cos(2\theta_{k,\pm}) \sin(\varepsilon_{k,\pm} t)$ and $B_\pm \equiv \sin(2\theta_{k,\pm}) \sin(\varepsilon_{k,\pm} t)$. Here, we have added extra indices $\pm$ for $\theta$ and $\varepsilon$ to indicate the evolutions driven by different Hamiltonians $H_{k,\pm,\varepsilon}$. It is straightforward to extend this result to Hahn echo:

$$
L_{\text{SE}}(t) = |\text{Tr}[|\uparrow\rangle \langle \downarrow| e^{-iH_{\varepsilon}/2}\sigma^z e^{-iH_{\varepsilon}/2} \rho \otimes |\psi\rangle \langle |\psi| e^{iH_{\varepsilon}/2}\sigma^z e^{iH_{\varepsilon}/2}]|
$$

$$
= |\text{Tr}[e^{-iH_{\varepsilon} t/2} e^{-iH_{\sigma^z} t/2} \rho e^{iH_{\varepsilon} t/2} e^{iH_{\sigma^z} t/2}]|
$$

$$
= \prod_{k > 0} \text{Tr}[\rho_k U_{k,\varepsilon}(t/2)U_{k,-}(t/2)U_{k,+}(t/2)U_{k,-}(t/2)].
$$ (A.12)

The decoherence presented in figures 1 and 2 is calculated by exact diagonalization of the bath Hamiltonian.

**Appendix B. Noise spectra**

To better understand the decoherence, we examine the noise spectra of the local field fluctuations. Fluctuation of the effective field $B = 2g \sum_{j=1}^N \sigma^z_j$ felt by the probe spin causes decoherence of the probe spin. The local field fluctuation has the correlation function $C(t) = \langle \tilde{B}(t) \tilde{B}(0) \rangle - \langle \tilde{B}(t) \rangle \langle \tilde{B}(0) \rangle$ where $\tilde{O}(t) \equiv e^{iHt} \tilde{O} e^{-iHt}$. The noise spectrum is
Figure B.1. Noise spectrum approach to the probe spin decoherence problem. Panels (a) and (b) show, respectively, the noise spectra of the quantum fluctuation at zero temperature ($\beta = \infty$) and finite temperature ($\beta = 1$) for different external fields $\lambda$. Panels (c) and (d) show, respectively, the filter functions for the FID and spin echo for different times. Panels (e) and (f) compare the decoherence obtained by the noise spectrum approach and the exact solution for $\beta = \infty$ and 1, respectively.

$$S(\omega) \equiv \int C(t) \exp(i\omega t) \, dt.$$  
In Gaussian noise approximation, the decoherence is determined by the noise correlation as

$$L_\alpha(t) = \exp \left[ -\frac{1}{2} \int_0^t \int_0^{t'} C(t_1 - t_2) f_\alpha(t_1) f_\alpha(t_2) \, dt_1 \, dt_2 \right], \quad \text{(B.1)}$$

where the modulation functions $f_{\text{FID}}(t') = 1$ in the case of FID; $f_{\text{SE}}(t') = 1$ for $t' \in [0, t/2]$ and $f_{\text{SE}}(t') = -1$ for $t' \in [t/2, t]$ in the case of spin echo. Since $\sum_{j=1}^N \sigma_j^2 = 2 \sum_{k \geq 0} \left[ \cos(2\theta_k)(b_k^\dagger b_k + b_k b_{-k}^\dagger - 1) - i \sin(2\theta_k)(b_{-k} b_k^\dagger + b_{-k}^\dagger b_k^\dagger) \right]$, we obtain the thermal fluctuation.
Figure B.2. FID evaluated at different finite temperatures for (a) $\beta = 50$, (b) $\beta = 10$, (c) $\beta = 5$ and (d) $\beta = 2$. The number of spins in the transverse-field Ising model is $N = 10000$ and the probe–bath coupling $g = 0.01$. In the FID of the probe spin, the sharp dip at the quantum critical point gradually disappears as the temperature increases.

which gives the noise at zero frequency with amplitude

$$C(0) = 16g^2 \sum_{k \geq 0} \frac{\exp(-\beta \epsilon_k)}{[1 + \exp(-\beta \epsilon_k)]^2} \cos^2(2\theta_k).$$  \hspace{1cm} \text{(B.2)}$$

The quantum fluctuation part gives the noise spectrum

$$S_Q(\omega) = 2\pi \sum_{k \geq 0} \delta(\omega - 2\epsilon_k) \frac{1 + \exp(-2\beta \epsilon_k)}{[1 + \exp(-\beta \epsilon_k)]^2} 8g^2\sin^2(2\theta_k)$$

$$= \begin{cases} 4g^2N \frac{[1 + \exp(-\beta \omega)]}{[1 + \exp(-\beta \omega/2)]^2} \frac{\sqrt{4\lambda^2 - (1 + \lambda^2 - \omega^2/16)^2}}{\lambda^2 \omega}, & \omega \in [4 |1 - \lambda|, 4 |1 + \lambda|], \\ 0, & \text{else}. \end{cases} \hspace{1cm} \text{(B.3)}$$
The decoherence of the probe spin is

\[ L_\omega(t) = \exp \left[ -\int_0^t \int_0^t C(0) f_\omega(t_1) f_\omega(t_2) \, dt_1 \, dt_2 \right] \exp \left[ -\int \frac{d\omega}{2\pi} S_Q(\omega) \frac{|F_\omega(\omega t)|^2}{\omega^2} \right] \tag{B.4} \]

in which the filter function \( \omega^{-2} |F_{\text{FID}}(\omega t)|^2 = 4\omega^{-2} \sin^2(\omega t/2) \) for FID and \( \omega^{-2} |F_{\text{SE}}(\omega t)|^2 = 16\omega^{-2} \sin^4(\omega t/4) \) for spin echo. And by using the scaled frequency (\( \omega = \omega t \)), the filter function can be expressed as \( M_{\text{FID}}(x) = \frac{1}{16} x^2 \sin^2(x/4) \) and \( M_{\text{SE}}(x) = \frac{1}{16} x^2 \sin^4(x/4) \), and the probe spin decoherence is reformulated as

\[
\ln |L_{\text{FID}}(t)| = -C(0)t^2 - t \int_0^\infty \frac{dx}{2\pi} S_Q(x/t) M_{\text{FID}}(x), \tag{B.5a}
\]

\[
\ln |L_{\text{SE}}(t)| = -t \int_0^\infty \frac{dx}{2\pi} S_Q(x/t) M_{\text{SE}}(x). \tag{B.5b}
\]

The noise spectrum approach is verified by comparison with the exact solution as shown in figure B.1. The noise spectra of the transverse-field Ising model are determined by the quasi-particle excitation spectra. At the critical point (\( \lambda = 1 \)), the noise spectra are gapless (figures B.1(a) and (b)). The spin decoherence is determined by the noise spectrum and the filter functions (figures B.1(c) and (d)). The spin echo filters out the zero-frequency component of the noise. As time increases, the filter function has greater low-frequency pass (figure B.1(d)). The noise spectrum method provides a good approximation of the decoherence (figures B.1(e) and (f)).

From equations (B.2)–(B.5), we see that the thermal noise (which leads to the Gaussian decay \( e^{-t^2} \)) dominates the FID when the temperature increases. The critical feature at the critical point, which comes from the quantum fluctuation, is blurred with increasing temperature (figure B.2). The quantum effect is therefore concealed by the thermal fluctuation at high temperature.

The magnetic susceptibility is evaluated by

\[
\chi = -N^{-1} \partial_\beta \sum_{i=1}^N \langle \sigma_i^z \rangle = -2N^{-1} \partial_\beta \sum_{k \geq 0} \frac{1 - e^{\beta \epsilon_k}}{1 + e^{\beta \epsilon_k}} \cos(2\theta_k). \tag{B.6}
\]

By Fourier transform of equation (3), we obtain the susceptibility as

\[
\chi = \frac{\beta}{2} C(0) + \int \frac{d\omega}{2\pi} S_Q(\omega) \frac{F_\chi(\beta \omega)}{\omega}. \tag{B.7}
\]

\( S_Q \) has the same definition as in equation (B.3). \( \omega^{-1} F_\chi(\beta \omega) \) is the corresponding filter function defined as

\[
\frac{F_\chi(\beta \omega)}{\omega} = \frac{1 - e^{-\beta \omega}}{\omega(1 + e^{-\beta \omega})}. \tag{B.8}
\]

After scaling the frequency by \( x = \omega \beta \), we obtain

\[
\chi(\beta) = \frac{\beta}{2} C(0) + \int_0^\infty S_Q \left( \frac{x}{\beta} \right) M_\chi(x) \frac{dx}{2\pi} \tag{B.9}
\]

with \( M_\chi(x) = x^{-1} \tanh (x/2) \) being the corresponding filter function.

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Figure C.1. Spin echo signals of a probe at infinite temperature as functions of the external field $\lambda$. The number of spins in the transverse-field Ising model is $N = 10\,000$. The probe–bath coupling is (a) $g = 0.01$ and (b) $g = 0.05$.

Appendix C. Finite probe–bath coupling effect

The probe spin decoherence (at external field $\lambda$) shows the difference between the quantum state evolutions of the system at different sides of the external field (namely at $\lambda + g$ and $\lambda - g$), which is also a reason why the probe spin decoherence is greatly enhanced at the critical point ($\lambda = 1$). Therefore, the larger probe strength leads to a broader transition region. The finite probe–bath coupling leads to a finite transition region near the critical point (figure C.1). To clearly resolve the critical point, it is desirable to have weak probe–bath coupling.

Appendix D. Revivals in free-induction decay

The FID of the probe spin coherence presents revival features in the paramagnetic phase ($\lambda > \lambda_c$). This phenomenon results from the finite and uniform coupling between the probe
Figure D.1. Revivals in the probe spin FID at infinite temperature. The calculation is performed with the number of spins in the bath $N$ and the probe–bath coupling $g$ being (a) $N = 50, g = 0.01$; (b) $N = 200, g = 0.01$; and (c) $N = 200, g = 0.02$. The FID presents revivals in the paramagnetic phase with periods $2\pi/(4g)$. 

and the finite number of bath spins. It can be understood by considering the limiting case of an infinite magnetic field in which the bath eigenstates have all spins quantized along the $z$-axis. As the probe–bath coupling $g$ is uniform for all the bath spins, the random local field takes integer multiples of $g$ and the decoherence by the thermal fluctuation presents periodic revivals with period $2\pi/(4g)$. With decreasing magnetic field, the bath spin quantization along the field direction is less perfect and the revival becomes less pronounced with the period increasing and eventually disappears at the ordered phase. Such a feature in FID may also
be used to determine the quantum critical point at high temperature for a finite-size system with uniform probe–bath coupling. For macroscopic systems or for non-uniform probe–bath coupling, however, the revival would be absent. In the study presented in figures 1 and 2, we consider timescales shorter than the revival period.

Appendix E. Numerical simulation of a dipolar spin-ring model

In the model system studied in section 5, the bath contains $N$ electron spin-(1/2)s placed evenly in a ring. The probe is a spin located below the center of the ring. A magnetic field $B$ is applied perpendicular to the ring (along the $z$-direction). To be specific, we assume that the probe spin is the spin of a NV center in diamond, which can be controlled and measured by optically detected magnetic resonance [48]. The spin ring can be made of electron spins placed on the diamond surface. The spins have dipolar coupling. The probe–bath Hamiltonian is given by

$$ H = \sum_{i=0}^{N} \gamma_e B S^z_i + \Delta (S^z_0)^2 $$

$$ + \sum_{i>j}^{N} \frac{\mu_0 \gamma_e^2}{4\pi R_{ij}^3} [S_i \cdot S_j - 3 R_{ij}^{-2} S_i \cdot R_{ij} R_{ij} \cdot S_j], $$

(E.1)

where $S_0$ is the spin-1 of the NV center electron at $R_0 = (x_0, y_0, z_0)$, $S_{i>0}$ is the $i$th bath spin at $R_i = (x_i, y_i, z_i)$, $\gamma_e = 1.76 \times 10^{11}$ rad s$^{-1}$ T$^{-1}$ is the gyromagnetic ratio of an electron spin, $\Delta = 2.87$ GHz is the zero-field splitting of the NV center spin and $R_{ij} = R_i - R_j$. In the nearest-neighbor approximation (as in calculation for figure 5) the coupling between non-neighboring bath spins ($|i-j| > 1$) is neglected. Since the zero-field splitting $\Delta$ is much greater than the probe–bath interaction ($\sim$ MHz), the flipping between the NV center spin state $|0\rangle$ and $|\pm 1\rangle$ is negligible. The model is reduced to a pure dephasing model. When the transition of the NV center spin $|0\rangle \leftrightarrow |+1\rangle$ is used to probe the quantum criticality of the bath, the effective Hamiltonian is given by

$$ H \approx H^{(0)} \otimes |0\rangle \langle 0| + H^{(+1)} \otimes |+1\rangle \langle +1|, $$

(E.2a)

$$ H^{(0)} = H_{\text{bath}}, $$

$$ H^{(+1)} = \gamma_e B + \Delta + H_{\text{bath}} + H_{\text{int}}, $$

(E.2b)

$$ H_{\text{bath}} = \sum_{i=1}^{N} \gamma_e B S^z_i $$

$$ + \sum_{i>j}^{N} \frac{\mu_0 \gamma_e^2}{4\pi R_{ij}^3} [S_i \cdot S_j - 3 R_{ij}^{-2} S_i \cdot R_{ij} R_{ij} \cdot S_j], $$

(E.2c)

$$ H_{\text{int}} = \sum_{j=1}^{N} \frac{\mu_0 \gamma_e^2}{4\pi R_{0j}^3} [S^z_j - 3 R_{0j}^{-2} z_0 j R_{0j} \cdot S_j], $$

(E.2d)
where \( z_{0j} = z_0 - z_j \). For two bath spins \( S_i \) and \( S_j \), if we choose the direction of \( R_{ij} \) as the \( Z \)-axis and the other two orthogonal directions as the \( X \)- and \( Y \)-axis, the spin interaction between them can be written as

\[
H_{ij} = -\frac{\mu_0 J}{4\pi} R_{ij}^2 \left( 2S_i^Z S_j^Z - S_i^X S_j^X - S_i^Y S_j^Y \right). 
\]  
(E.3)

This has the form of XXZ interaction. If only the nearest-neighbor coupling is taken into account and the ring is large enough (so that \( R_{i(i+1)} \) and \( R_{(i-1)i} \) are almost parallel), the dipolar spin-ring model reduces to the XXZ model \[33\].

The NV center spin is initially in a coherent state \( |0\rangle + |+1\rangle \), and the bath is initially in a thermal equilibrium state described by a density matrix \( \rho = Z^{-1} e^{-\beta H_{\text{bath}}} \) with the normalization factor \( Z = \text{Tr}[e^{-\beta H_{\text{bath}}}]. \) The coherence of the NV center spin in the case of FID at time \( t \) is

\[
L_{\text{FID}}(t) = |\text{Tr}[e^{-iH^{(0)}t} \rho e^{iH^{(1)}t}]| \]  
(E.4)

and the spin echo is

\[
L_{\text{SE}}(2t) = |\text{Tr}[e^{-iH^{(1)}t} e^{-iH^{(0)}t} \rho e^{iH^{(1)}t} e^{iH^{(0)}t}]| \]  
(E.5)

The spin correlation in figure 5 is defined between two bath spins at the endpoints of a diameter of the ring.

\[
C(1, N/2 + 1) = \text{Tr}[\rho S_1 \cdot n_1 S_{N/2+1} \cdot n_{N/2+1}], 
\]  
(E.6)

where \( n_1 \) and \( n_{N/2+1} \) are the unit vectors along the tangential directions of the ring at the positions \( R_1 \) and \( R_{N/2+1} \), respectively.

The low-energy states of the spin bath are calculated by the Lanczos algorithm \[49\]. Tens of lowest eigenenergies and corresponding eigenstates of \( H_{\text{bath}} \) are numerically obtained. The convergence of the solution has been tested.

The time evolution \( e^{-iH^{(0)}t} \) or \( e^{-iH^{(1)}t} \) and the density matrix \( e^{-\beta H_{\text{bath}}} \) are calculated by the Chebyshev polynomial expansion \[50–52\]. For a time-independent Hamiltonian, the evolution operator \( U(t) = \exp(-iHt) \) is expanded by the Chebyshev polynomials of the operator \( G \equiv H/E_0 \), where \( E_0 \) is a rescaling factor which makes the absolute values of all the eigenvalues of \( G \) less than one \[50\]. After this rescaling, the evolution operator is expanded by

\[
U(t) = \exp(-i\tilde{t}G) = J_0(\tilde{t}) + 2 \sum_{k=1}^{\infty} (-i)^k J_k(\tilde{t}) T_k(G), 
\]  
(E.7)

where \( \tilde{t} = E_0 t \) is the dimensionless rescaled time, \( J_k(\tilde{t}) \) is the \( k \)-th order Bessel function of the first kind and \( T_k(G) \) are the Chebyshev polynomials of the operator \( G \). In practice, a truncation at \( k = 1, 5\tilde{t} \) already gives a precision of \( 10^{-7} \) or better \[50\].

At infinite temperature, the density matrix \( \rho = 2^{-N} I \) is proportional to a unity matrix, and we can approximate the trace \( \text{Tr} [...] \) by averaging the expectation values over \( M \) samples of states \( M^{-1} \sum_{m=1}^{M} \langle \psi_m | ... | \psi_m \rangle \), where \( |\psi_m \rangle \) is a normalized random bath state. In the basis of the direct-product states \( |Y_a\rangle \) of \( N \) bath spins, \( |\psi_m \rangle = \sum_{a=1}^{2^N} C_a |Y_a\rangle \), where \( C_a \) are independent, uniformly distributed random complex numbers satisfying the normalization condition \( \sum_{a=1}^{2^N} |C_a|^2 = 1 \). For a sufficiently large number of bath spins (\( N > 12 \)), a single realization of \( C_a \) (\( M = 1 \)) is sufficient to precisely calculate decoherence at infinite temperature \[51\].
Figure E.1. Test of the nearest-neighbor dipolar interaction approximation. Panels (a)–(c) are in turn the 20 lowest eigenenergies, spin correlations (at various inverse temperatures indicated by values of $\beta$) and spin echo signal (at infinite temperature) calculated with the full-interaction Hamiltonian. Correspondingly, panels (d)–(f) are similar to (a)–(c) but calculated with the nearest-neighbor dipolar interaction approximation. The dashed lines denote the critical external fields. The spin ring has a radius of 15 nm and the probe spin is 5 nm below the center of the ring.

To calculate the properties at finite temperature, an evolution operator along an imaginary-time axis (inverse-temperature axis) is defined as $\mathcal{U}(\beta) = \exp(-\beta H)$. The evolution operator is again calculated by the Chebyshev polynomial expansion

$$\mathcal{U}(\beta) = \exp(-\tilde{\beta} G) = I_0(\tilde{\beta}) + 2 \sum_{k=1}^{\infty} (-1)^k I_k(\tilde{\beta}) T_k(G), \quad (E.8)$$

where $\tilde{\beta} = E_0\beta$ is the dimensionless rescaled inverse temperature and $I_k(\tilde{\beta})$ is the $k$th-order modified Bessel function of the first kind. In contrast to the case of infinite temperature, to evaluate the trace $\text{Tr}[\ldots]$, we need thousands of random samplings to obtain the converged results, because the imaginary-time evolution operator $\mathcal{U}(\tilde{\beta})$ puts most of the weight on the eigenstates with lower energies [52]. The lower the temperature, the more the samplings that
are needed. In the case of extreme low temperature, we switch to a direct calculation of
\[ \exp(-\beta H) = \sum_n \exp(-\beta E_n) |n\rangle \langle n|, \]
because only several eigenstates with lowest energies are relevant, which we have obtained by the Lanczos algorithm.

In section 5, we simulate the decoherence of the probe spin coupled to the bath of 20 spins with the nearest-neighbor approximation. To test the validity of this approximation, we compare calculation with the full-interaction Hamiltonian and that with the nearest-neighbor approximation for a bath of 16 spins. The results in figure E.1 show that the nearest-neighbor approximation describes the system very well except that the critical external field is shifted from 0.152 G in (a)–(c) to 0.112 G in (d)–(f).

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