Numerical modeling of the central spin problem using the spin coherent states
P-representation

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In this work, we consider decoherence of a central spin by a spin bath. In order to study the non-perturbative decoherence regimes, we develop an efficient mean-field-based method for modeling the spin-bath decoherence, based on the P-representation of the central spin density matrix. The method can be applied to longitudinal and transversal relaxation at different external fields. In particular, by modeling large-size quantum systems (up to 16000 bath spins), we make controlled predictions for the slow long-time decoherence of the central spin.

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Detailed understanding of the decoherence of various quantum systems is important for many areas, from quantum optics and solid-state physics to the quantum information processing, where decoherence constitutes a major obstacle for building a practical quantum computer. For example, in a quantum dot-based architecture, the quantum bit is represented by a spin of a single electron (central spin) placed in a quantum dot (QD). Due to interaction with the bath of nuclear spins in a QD, the electron spin quickly “looses memory” about its initial orientation and can not be used for computation.

Experimental studies of this process has become possible very recently [1, 2], and detailed theoretical understanding of the experimental results is timely and important. Moreover, the problem of a central spin coupled to the spin bath [3] (the “quantum central spin problem”) has recently arisen in other contexts (decoherence in magnetic molecules, dynamics of the cold fermions pairing), and has attracted much attention.

Decoherence is a complex quantum many-body phenomenon, and satisfactory solutions can be obtained only in very special cases [4, 5]. Perturbation theory can be successfully applied in the case of a strong magnetic field or polarized nuclear spin bath (which produces a strong Overhauser field acting on the central spin) [6, 7]. But for the experimentally important non-perturbative regimes, no well-justified method, numerical or analytical, has been suggested yet. The static approximation [8, 9, 10], which simply neglects the dynamics of the bath spins, works only at short times, while the interesting long-time dynamics of the central spin remains an open problem, and the simulations on moderate-sized systems (~20 spins) do not give conclusive results.

In this work, we present a novel approach to the quantum central spin problem based on the time-dependent mean field (TDMF) theory. It has been pointed out previously [10, 11] that the mean field approach should be adequate, since the central spin interacts with a large number $N$ of the bath spins (loosely speaking, the number of the “nearest neighbors” for the central spin is large, i.e. the coupling of the central spin with the bath has an infinite range). However, the standard mean field approach [12] gives a clearly wrong answer (see below). We use the spin coherent state P-representation [13] to modify the standard TDMF, and present an efficient approach, which gives excellent agreement with the exact solution of the many-spin quantum problem already for rather small systems (up to 20 spins). By applying this method to large-scale problems, we study the interesting long-time dynamics of the central spin. Moreover, the P-representation approach allows us to understand why the properly corrected TDMF theory works for large $N$, and what the limitation of the method are.

It is interesting to point out that the spin coherent states are traditionally used in the spin path integrals and in the semiclassical approximation for quantum spins. The powerful methods based on P- and Q-representations, so useful in quantum optics, have not been widely applied to the spin systems studies. We expect that this work will help developing novel coherent-state approaches to studying spin systems. Another interesting point concerns the basic ideas of the mean field theory. The standard mean field theory approximates, in the optimal way, the exact many-spin wavefunction as a product of single-spin wavefunctions. However, when studying decoherence, we are only interested in the state of the central spin, not the whole many-body state. It is interesting that there is a justified modification of the standard TDMF (presented below) which provides a much better approximation for the relevant observables (the state of the central spin) at the expense of irrelevant information (the state of the bath).

The electron spin in a QD interacting with the bath of $N$ nuclear spins can be described by the Hamiltonian

\begin{equation}
H = g_s \mu_B B_0 S_0^z + \sum_{k=1}^{N} A_k S_k S_0 = H_0^z S_0^z + \sum_{k=1}^{N} H_k \tag{1}
\end{equation}

\[H_0^z = g_s \mu_B B_0 S_0^z + \sum_{k=1}^{N} A_k S_k S_0\]
where \( \mathbf{S}_0 = (S^x_0, S^y_0, S^z_0) \) are the operators of the electron spin, \( \mathbf{S}_k \) are the operators of the bath spins, and \( A_k = (8\pi/3)g_\mu_B g_n \mu_n |\Psi(x_k)|^2 \) is the contact hyperfine coupling which is determined by the electron density \( |\Psi(x_k)|^2 \) at the site \( x_k \) of the \( k \)-th nuclear spin and by the Landé factors of the electron \( g_\mu \) and of the nuclei \( g_n \). The first term in Eq. 1 describes the Zeeman energy of the electron spin in the external magnetic field \( B_0 \), and the second term represents the contact hyperfine coupling. The omitted terms, such as the Zeeman energy of the nuclear spins and the non-isotropic part of the hyperfine coupling, are very small and can be neglected for a wide range of experimental situations. Eq. 1 is the standard Hamiltonian of the quantum central spin problem \( \mathbf{H} \).

We are interested in the dynamics of the central spin, i.e. in the dynamics of \( \mathbf{s}_0(t) = \text{Tr}\rho(t)\mathbf{S}_0 \), where \( \rho(t) \) is the density matrix of the total system (central spin plus the bath). Although the quantum central spin problem is integrable, the formal solution \( [3] \) is very complex, and, the bath). Although the quantum central spin problem is integrable, the formal solution \( [3] \) is very complex, and, to our knowledge, it has not been used for actual calculations of \( \mathbf{s}_0(t) \), neither analytically, nor numerically. Efficient approximate approaches are needed, and the TDMF theory is a natural first step. Within the mean-field approach, we approximate the wavefunction \( |\Psi\rangle \) of the total system as a product \( |\Psi\rangle = |\psi_0\rangle \bigotimes_{k=1}^{N} |\psi_k\rangle \) of the single-spin wavefunctions \( |\psi_j\rangle \). The TDMF equations of motion for \( |\psi_j\rangle \) are obtained by substituting this ansatz into the Dirac’s functional \( D = \int dt \langle \psi_j | d\psi /dt | - \mathcal{H} | \psi_j \rangle \), and requiring that \( \delta D = 0 \) with respect to small variations of all \( |\psi_k\rangle \). The resulting equations of motion can be presented in a simple form as

\[
\dot{s}_j = [\mathbf{h}_j \times \mathbf{s}_j] \quad (j = 0 \ldots N) \tag{2}
\]

\[
\mathbf{h}_0 = H_0 \mathbf{e}_z + \sum_k A_k \mathbf{s}_k, \quad \mathbf{h}_k = A_k \mathbf{s}_0 \quad (k = 1 \ldots N) \tag{3}
\]

where \( \mathbf{s}_j = \text{Tr}\rho(t)\mathbf{S}_j \), and \( [\mathbf{h}_j \times \mathbf{s}_j] \) is the vector product of \( \mathbf{h}_j \) and \( \mathbf{s}_j \). The physical meaning of these equations is simple: every \( j \)-th spin precesses in its own time-dependent effective field \( \mathbf{h}_j \) given by Eq. 3. However, TDMF theory gives a very bad approximation to the exact solution of the problem. It can be seen, for example, from comparison of the standard TDMF theory with the exact numerical solutions \( [3] \) for several distributions of \( A_k \) (see Fig. 2): the disagreement is significant.

In order to construct a working approximation based on the TDMF, let us consider the P-representation of the system’s density matrix in the basis of spin coherent states \( [13, 15] \). The spin coherent state for spin \( J \) is defined as \( |\mu\rangle = N^{-1/2} \sum_{m=0}^{2J} [ (2J)! / (m! (J-m)!) ]^{1/2} \mu^m |J-m\rangle \), where \( N = (1 + |\mu|^2)^{-J} \) is the normalization constant. For a spin 1/2, the coherent state has a simple form \( |\mu\rangle = \cos(|\mu|/2) \uparrow + \sin(|\mu|/2)e^{i\theta} \downarrow \), where we used the parametrization \( \mu = \tan(\theta/2)e^{i\phi} \). The basis of coherent states is overcomplete, and by choosing an appropriate real-valued function \( \hat{A}(\theta, \phi) \), any hermitian operator \( \mathcal{A} \) can be represented in a diagonal form: \( \mathcal{A} = \int_0^{2\pi} \hat{A}(\theta, \phi)|\mu\rangle \langle \mu| \sin \theta d\theta d\phi \), where the integration is performed over the sphere. Note that \( \hat{A}(\theta, \phi) \neq \langle \theta, \phi | \mathcal{A} | \theta, \phi \rangle \). Moreover, the function \( \hat{A}(\theta, \phi) \) is not uniquely determined; if we add to it any linear combination of the spherical harmonics \( Y^m_l (\theta, \phi) \) of the order \( l > 2J \), then the value of the integral remains the same, and the new function would define the same operator \( \mathcal{A} \). Obviously, the many-spin density matrix \( \rho \) can also be written in the diagonal form:

\[
\rho(t) = \int p(\{\theta_j, \phi_j\}, t) \bigotimes_{j=0}^{N} |\mu_j\rangle \langle \mu_j| \prod_{j=0}^{N} \sin \theta_j d\theta_j d\phi_j. \tag{4}
\]

with a real-valued function \( p(\{\theta_j, \phi_j\}, t) \), where \( \{\theta_j, \phi_j\} \) is the set of all \( \theta_0, \ldots, \theta_N \) and \( \phi_0, \ldots, \phi_N \). This representation for the density matrix is called the P-representation \( [13] \). Note that the operator part of the expression (4) has a mean-field form, i.e. it is a product of single-spin density matrices \( |\mu_j\rangle \langle \mu_j| \). In P-representation, the quantum-mechanical average \( x = \text{Tr}(\rho(t)X) \) of any observable \( X \) can be calculated by a simple formula

\[
x = \int p(\{\theta_j, \phi_j\}, t) \bigotimes_{j=0}^{N} |\mu_j\rangle \langle \mu_j| X |\mu_j\rangle \prod_{j=0}^{N} \sin \theta_j d\theta_j d\phi_j. \tag{5}
\]

Our goal is to model the evolution of the function \( p(\{\theta_j, \phi_j\}, t) \). However, the direct solution of the complex partial differential equation for \( p(\{\theta_j, \phi_j\}, t) \) is impossible for a large (hundreds or more) number of spins, and we use a different approach. We note that if \( p(\{\theta_j, \phi_j\}, t) \geq 0 \) then this function can be interpreted as a probability for the system to be in the product state \( |\Psi\rangle = \bigotimes_{j=0}^{N} |\mu_j\rangle \), and we need to simulate the dynamics of the probability distribution \( p(\{\theta_j, \phi_j\}, t) \). To do that, we initially generate many realizations of the random vector \( (\theta_0^m, \ldots, \theta_N^m, \phi_0^m, \ldots, \phi_N^m) \) distributed according to the probability distribution \( p(\{\theta_j, \phi_j\}, 0) \) (the index \( m = 1, \ldots, M \) enumerates the different realizations). Then we propagate every initial vector \( (\theta_0^m, \ldots, \theta_N^m, \phi_0^m, \ldots, \phi_N^m) \) in time, so that after a lapse of time \( t \), the initial vector evolves into a vector \( (\Theta_0^m(t), \ldots, \Theta_N^m(t), \Phi_0^m(t), \ldots, \Phi_N^m(t)) \). If the equations of motion for all the variables \( \Theta_j^m(t) \) and \( \Phi_j^m(t) \) are chosen correctly, then the function \( p(\{\theta_j, \phi_j\}, t) = p(\Theta_j(t), \Phi_j(t)) \), and the value \( x = \text{Tr}(\rho(t)X) \) of any observable \( X \) can be calculated as an average over all realizations; \( x = \frac{1}{M} \sum_{m=1}^{M} \sin \Theta_j^m(t) \bigotimes_{j=0}^{N} |\Theta_j^m\rangle \langle \Theta_j^m| \bigotimes_{j=0}^{N} |\Phi_j^m\rangle \langle \Phi_j^m| X |\Theta_j^m\rangle \langle \Phi_j^m| \). To implement this approach, we need to determine the equations of motion for \( \Theta_j(t), \Phi_j(t) \) which would produce a good approximation for \( p(\{\theta_j, \phi_j\}, t) \). As a first step, let us find the exact equations of motion for \( p(\{\theta_j, \phi_j\}, t) \). For simplicity, let us study one term in the
central-spin Hamiltonian \( H \), i.e., we consider two spins 1/2 (the central spin and the \( k \)-th bath spin) coupled by the isotropic Heisenberg interaction \( H_k = A_k \sigma_k^x \sigma_k^x \).

The most general form for the two-spin density matrix is
\[
\rho = w_{00} 1_0 1_k + w_{01} 1_0 \sigma_k^z + w_{10} \sigma_0^z 1_k + w_{11} \sigma_0^z \sigma_k^z,
\]
where \( \sigma_0^z \) and \( \sigma_k^z \) denote the Pauli matrices for the 0-th and the \( k \)-th spin, respectively. Here and below, we assume summation over the repeating indices. From the von Neumann’s equation \( \dot{\rho}(t) = i[\rho(t), H] \), we obtain \( \dot{w}_{00}(t) = 0 \) (which expresses that \( \text{Tr}\rho(t) = 1 \)), and
\[
\dot{w}_{0\gamma}(t) = \frac{A_k}{\gamma} \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), \quad \dot{w}_{\gamma 0}(t) = -\frac{A_k}{\gamma} \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t),
\]
where \( \epsilon_{\alpha\beta\gamma} \) is a completely antisymmetric unity tensor (permutation symbol). These equations of motion determine the dynamics of \( p\{\theta_0, \phi_0, \theta_k, \phi_k\} \), \( t \). From the P-representation \( p \) it follows that \( p\{\theta_0, \phi_0, \theta_k, \phi_k\} = p_{00}(t) + p_{0\gamma}(t) \sigma_k^x + p_{\gamma 0}(t) \sigma_0^x \sigma_k^x \), where
\[
p_{00} = \left(1/\pi^2\right) w_{00}, \quad p_{0\gamma} = \left(3/\pi^2\right) w_{0\gamma}, \quad p_{\gamma 0} = \left(3/\pi^2\right) w_{\gamma 0}, \quad P_{11} = \left(3/\pi^2\right) w_{11},
\]
and \( p_{0\gamma}(t) \) is the same function of \( t \). Here, we use the shorthand notation \( C_0 = \sin \theta_0 \cos \phi_0, C_1 = \sin \theta_0 \sin \phi_0, C_2 = \cos \theta_0 \) (and similarly for \( C_{0k}, C_{1k}, C_{2k} \)). The spherical harmonics of the order higher than one can also be added to \( p\{\theta_0, \phi_0, \theta_k, \phi_k\} \), but they do not change the density matrix \( \rho \), and therefore are not physically significant.

The mean-field structure of the P-representation for the density matrix (Eq. 4) suggests that the equations of motion for \( \{\Theta_0(t), \Phi_0(t), \Theta_k(t), \Phi_k(t)\} \) should also have a mean-field form corresponding to Eq. 2 but the local fields should be re-defined to provide optimal approximation for \( S_0(t) \). For simplicity, we omit the discussion of the general form for \( H_0(t) \) and \( H_k(t) \), and proceed to the answer. We introduce the shorthand notation
\[
C_0' = \sin \Theta_0 \cos \Phi_0, C_1' = \sin \Theta_0 \sin \Phi_0, C_2' = \cos \Theta_0 \quad (\text{and similarly for } C_{0k}', C_{1k}', C_{2k}'),
\]
and postulate the following equations of motion for the density matrix \( \rho \):
\[
\dot{w}_{0\gamma}(t) = -g_2 \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), \quad \dot{w}_{\gamma 0}(t) = g_1 \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t),
\]
\[
\dot{w}_{\alpha\beta}(t) = \left(1/3\right) \epsilon_{\alpha\beta\gamma} [g_2 w_{0\gamma}(t) - g_1 w_{\gamma 0}(t)],
\]
(cf. Eqs. 6), and, trivially \( \dot{w}_{00}(t) = 0 \). The Eqs. 6 and 8 are incompatible for any \( g_1 \) and \( g_2 \) (i.e., TDMF is never exact). However, we are interested only in \( w_{\gamma 0}(t) \), since only this term determines the value of \( S_0(t) \). Therefore, we choose \( g_1 = g_2 = g = \frac{A_k \sqrt{3}}{2} \), and differentiate Eqs. 6 and 8 with respect to time once more. Then we see that both Eqs. 6 and 8 produce the same result:
\[
\dot{w}_{\gamma 0}(t) = -\dot{w}_{0\gamma}(t) = \left(\frac{A_k \sqrt{2}}{2}\right) w_{\gamma 0}(t),
\]
and that the functions \( w_{\gamma 0}(t) \) produced by the approximate equations 7 and by the exact equations 6 coincide, provided that the initial conditions \( w_{\gamma 0}(0) \) and \( \dot{w}_{\gamma 0}(0) \) also coincide. The latter condition is satisfied when all \( w_{\alpha\beta}(0) = 0 \), so the method described above is applicable only to unpolarized baths. On the other hand, for polarized baths, one can use the perturbational approaches 10, 11, so this limitation is not serious. Therefore, in order to fix the standard TDMF in case of spins 1/2, we just need to take Eqs. 6 and replace \( A_k \) by \( A_k \sqrt{3}/2 \).

It may seem that we just derived the standard semiclassical equations of motion, but this is not correct. For instance, if we take unequal spins 1 and 1/2 \( (S_0 = 1 \) and \( S_k = 1/2 \)) then the analysis above gives \( g_1 = A_k \sqrt{3}/2, g_2 = A_k \sqrt{7}/2 \), while the semiclassics would give \( g_1 = A_k \sqrt{3}/2, g_2 = A_k \sqrt{7}/2 \). Moreover, the initial conditions in our approach and in the semiclassical approach are different. For example, in case when the central spin 1/2 is initially directed along the z-axis, so that the initial density matrix \( \rho(0) = 2^{-N} |10\rangle\langle 10| \otimes \otimes_{k=1}^{N-1} 1 \), our approach requires \( p\{\theta_j, \phi_j\}, 0 = (4\pi)^{-N-1} (1 + 3 \cos \theta_0) \), while the semiclassical approximation would correspond to \( p\{\theta_j, \phi_j\}, 0 = (4\pi)^{-N-1} \delta(\cos \theta_0 - 1), \delta(\ldots) \) is the Dirac’s delta-function.

The approach developed above gives excellent results at both short and long times, for different distributions of the coupling constants \( A_k \), external fields \( H_0 \), and is applicable to both longitudinal and transversal relaxation. A small fraction of the representative test results for a moderate number of bath spins \( (N = 15 \) to 20) is shown in Figs. 1, 2, where we used the Chebyshev expansion method 14 for exact solution of the quantum problem. The longitudinal decay shown in Fig. 1 is typical; the long-time tail suggests the slow relaxation \( s_0(t) \sim 1/\ln t \),
pled to a bath of 16000 spins 1/2, field $H_0 = 1.0$. (a) central spin 1/2, $N = 21$ bath spins (b) central spin 1, $N = 19$ bath spins. Solid lines — exact solutions, open circles — our approximation; agreement is excellent. Dashed lines — standard TDMF; the disagreement with the exact solution is significant.

FIG. 3: Long-time relaxation of the central spin 1/2 couplings $A_k$ are randomly distributed between -0.4 and 0.6, field $H_0 = 1.0$. (a): central spin 1/2, $N = 21$ bath spins (b): central spin 1, $N = 19$ bath spins. Solid lines — exact solutions, open circles — our approximation; agreement is excellent. Dashed lines — standard TDMF; the disagreement with the exact solution is significant.

but the results are not conclusive, since for moderate-sized systems $s_0(t)$ for larger number of bath spins coupled to the central spin. Moreover, this assumption is well-supported by numerous numerical tests. In Fig. 5 we present the long-time longitudinal relaxation of an electron spin in a model QD: we assumed that the bath spins 1/2 are placed at the sites of a piece of a cubic lattice with the size $N_x 	imes N_y 	imes N_z$, ($N_x = N_y = 40$, $N_z = 10$, so the total number of bath spins $N = N_x N_y N_z = 16000$). The long-time relaxation is extremely slow, clearly demonstrating the law $1/\ln t$ (see Fig. 5). Our simulations show that the law $1/\ln t$ holds for unpolarized baths for different forms of the electron densities, i.e. for different distributions of $A_k$ (two examples are given in Fig. 5). Our approach also performs well (see Fig. 5) for an anisotropic X-Y coupling between the central and the bath spins $\mathcal{H} = H_0 S_0^z + \sum_k A_k (S_0^x S_k^x + S_0^y S_k^y)$, which is important for analyzing interesting experiments of Ref. 2. The results show good qualitative agreement with the experimental curves, but the experiments are performed with $\sim 5$–10% polarization, so that our model needs further development for rigorous quantitative comparison.

FIG. 4: Longitudinal relaxation $s_0(t)$ of the central spin 1/2 coupled to a bath of spins 1/2 via the anisotropic X-Y Hamiltonian, external field $H_0 = 1.0$. (a): $N = 21$ bath spin, $A_k$ are randomly distributed between 0 and 1.0. Solid line — exact solution, open circles — approximation. (b): $N = 2000$ spins, the couplings $A_k$ are the same as in Fig. 3, but for smaller lattice $N_x = N_y = 20$, $N_z = 5$.

FIG. 3: Long-time relaxation of the central spin 1/2 coupled to a bath of 16000 spins 1/2, field $H_0 = 0$. Graphs show $1/s_0^z(t)$ as a function of $\ln t$. The coupling constants were calculated as $A_k = (1/4)u(x_k)$, where the $u(x)$ is the electron density. (a): $u(x)$ is taken as a Gaussian with the half-widths $d_x = 8.4a$, $d_y = 9.1a$, $d_z = 2.2a$ ($a$ is the lattice parameter), shifted from the center of the lattice by the vector $(0.252a, 0.448a, 0.1a)$; (b): $u(x)$ is taken as an exponential function of $x$, with the same parameters. We used an extra averaging over 20 neighboring time points to decrease the number of realizations. The solid lines are obtained from raw data.

We considered the systems with $N = 1000$-15000 spins. For small $N = 2$–5, our approximation is very crude because the equations of motion lead to the appearance of higher-order spherical harmonics in the function $\rho(\theta, \phi, t)$ (the terms proportional to $e^{a_0^z l_0^x k^y k}$ etc.). These terms do not change the form of $\rho(t)$ (they disappear after integration in Eq. 3), but they affect the equations of motion for physically relevant terms, i.e. the actual equation of motion for $w_{\gamma,0}(t)$ becomes $\dot{w}_{\gamma,0}(t) = (A_k^2/2)(w_{\gamma,0} - w_{\gamma}) + V$, where $V$ is the contribution from the higher-order harmonics. However, the contribution of $V$ into $s_0(t)$ is bounded, and quickly decreases for larger $N$, so we expect our approximation for $s_0(t)$ to work the better the larger $N$ is. This is a natural expectation, since our method is based on TDMF, which works better for larger number of bath spins coupled to the central spin.

Summarizing, we used the spin coherent states $P$-representation to develop a novel approach to the quantum central spin problem, based on the time-dependent mean field theory. The approach gives excellent agreement with the exact solutions, and is valid for a wide range of systems and conditions. We use it to study the long-time longitudinal relaxation of the electron spin in a quantum dot, and find that the slow decay $1/\ln t$ is observed in different situations. Our approach provides an interesting extension of the mean-field theory, and is applicable to many-spin central systems as well.

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[16] Similar relaxation was found in [10] for 2-D Gaussian electron density, using adiabatic approximation applied to the semiclassical equations of motion. Accuracy of this method is unclear; it is supposed to be correct for large \( N \), but we can neither confirm nor reject that: the exact solution for more than \( \sim 20 \) bath spins is extremely difficult, while for \( N = 22 \) bath spins the exact solution disagrees with the approximation of Ref. [10]. Also, \( 1/\ln t \) was predicted from the perturbation theory for polarized baths [6] in case of 2-D dot with Gaussian electron density, but other forms of decay have been predicted for other electron density distributions. In our simulations for unpolarized baths, we see \( 1/\ln t \) for different electron density distributions.