

Numerical Modeling of the Central Spin Problem Using the Spin-Coherent-State 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 nonperturbative 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 transverse relaxation at different external fields. In particular, by modeling large-size quantum systems (up to 16 000 bath spins), we make controlled predictions for the slow long-time decoherence of the central spin.

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Detailed understanding of decoherence is important for many areas, from quantum optics and solid-state physics to quantum computation (QC). For example, in a quantum dot-based architecture for QC, the quantum bit is represented by a spin of a single electron (central spin) placed in a quantum dot. Due to interaction with the bath of nuclear spins in a dot, the electron spin quickly “loses memory” about its initial orientation and cannot be used for computation. Experimental studies of this process have become possible very recently [1,2], and detailed theoretical understanding of the experimental results is timely and important. Also, 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 BCS condensates) [4,5] and has attracted much attention.

Decoherence is a complex quantum many-body phenomenon, and satisfactory solutions can be obtained only in special cases [6,7]. 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) [8,9]. But for the experimentally important nonperturbative regimes, no well-justified method, numerical or analytical, has been suggested yet. The frozen-bath approximation [7,10,11] works only at short times, while the interesting long-time dynamics of the central spin remains an open problem.

Below, we present a novel approach to the quantum central spin problem based on time-dependent mean-field (TDMF) theory. It has been pointed out [5,12] that the mean-field approach should be adequate, since the central spin simultaneously interacts with a large number N of the bath spins (loosely speaking, the number of the “nearest neighbors” for the central spin is large). However, the standard TDMF [13] gives a bad approximation (see below). We use the spin-coherent-state P representation [14] 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, where exact simulations would be astronomically long, we study the interesting long-time dynamics of the central spin. Moreover, the P -representation approach allows us to understand why the corrected TDMF theory works for large N and what the limitations of the method are.

While 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 quantum spin systems. Another interesting point concerns the basic ideas of the mean-field theory. The standard TDMF approximates, in the optimal way, the exact many-spin wave function as a product of single-spin wave functions. However, when studying decoherence, we are interested only in the state of the central spin, not the whole many-body state, and there is a justified modification of the standard TDMF, presented below, which provides an excellent 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 interacting with a bath of N nuclear spins in a quantum dot is described by the Hamiltonian which includes the Zeeman energy of the electron spin in the external magnetic field B_0 and the contact hyperfine coupling:

$$\mathcal{H} = g_e^* \mu_B B_0 S_0^z + \sum_{k=1}^N A_k \mathbf{S}_k \mathbf{S}_0 = H_0 S_0^z + \sum_{k=1}^N \mathcal{H}_k, \quad (1)$$

where $\mathbf{S}_0 = (S_0^x, S_0^y, S_0^z)$ are the operators of the electron spin, \mathbf{S}_k are the operators of the bath spins, and $A_k = (8\pi/3)g_e^* \mu_B g_n \mu_n u(\mathbf{x}_k)$ is the contact hyperfine coupling which is determined by the electron density $u(\mathbf{x}_k)^2$ at the site \mathbf{x}_k of the k th nuclear spin and by the Landé factors of the electron g_e^* and of the nuclei g_n . The terms omitted in Eq. (1), such as the Zeeman energy of the nuclear spins, the

anisotropic part of the hyperfine coupling, etc., are very small and can be neglected in many experimental situations. Equation (1) is the standard Hamiltonian of the quantum central spin problem [3].

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, to our knowledge, it has not yet been used for actual calculations of $\mathbf{s}_0(t)$. Efficient approximate approaches are needed, and the TDMF theory is a natural first step: We approximate the wave function $|\Psi\rangle$ of the total system as a product $|\Psi\rangle = |\psi_0\rangle \otimes_{k=1}^N |\psi_k\rangle$ of the single-spin wave functions $|\psi_j\rangle$. The TDMF equations of motion (EOM) for $|\psi_j\rangle$ are obtained by substituting this ansatz into the Dirac's functional $D = \int dt \langle \Psi | i(d\Psi/dt) - \mathcal{H}\Psi$ and requiring $\delta D = 0$ with respect to variations of $|\psi_k\rangle$. The resulting EOM are

$$\dot{\mathbf{s}}_j = [\mathbf{h}_j \times \mathbf{s}_j] \quad (j = 0, \dots, N), \quad (2)$$

$$\mathbf{h}_0 = H_0 \mathbf{e}_z + \sum_k A_k \mathbf{s}_k, \quad \mathbf{h}_k = A_k \mathbf{s}_0 \quad (k = 1, \dots, N), \quad (3)$$

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 and strongly disagrees with the exact numerical solution [15]; see an example in Fig. 2.

To construct a working approximation based on the TDMF, we use the P representation of the system's density matrix in the basis of spin-coherent states [14]. The coherent state for spin J is defined as $|\mu\rangle = \mathcal{N} \sum_{m=0}^{2J} \{(2J)!/[m!(2J-m)!]\}^{1/2} \mu^m |J-m\rangle$, where $\mathcal{N} = (1+|\mu|^2)^{-J}$ is the normalization constant. For a spin $1/2$, the coherent state has a simple form $|\mu\rangle = \cos(\theta/2)|\uparrow\rangle + \sin(\theta/2)e^{i\phi}|\downarrow\rangle$, 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 $\tilde{A}(\theta, \phi)$, any Hermitian operator A can be represented in a diagonal form: $A = \int_{\Omega} \tilde{A}(\theta, \phi) |\mu\rangle \langle \mu| \sin\theta d\theta d\phi$, where the integration is performed over the sphere [16]. The diagonal representation of the many-spin density matrix ρ via a real-valued function $p(\{\theta_j, \phi_j\}, t)$,

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

is called the P representation [14] ($\{\theta_j, \phi_j\}$ denotes the set of all $\theta_0, \dots, \theta_N$ and ϕ_0, \dots, ϕ_N). In the P representation, the quantum-mechanical average $x = \text{Tr}[\rho(t)X]$ of any observable X can be calculated simply

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

Our goal is to model the evolution of the function $p(\{\theta_j, \phi_j\}, t)$, but the direct solution of the complex partial differential equation for $p(\{\theta_j, \phi_j\}, t)$ is impossible for large N . Instead, 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 $(\theta_0^{(m)}, \dots, \theta_N^{(m)}, \phi_0^{(m)}, \dots, \phi_N^{(m)})$ distributed according to the probability distribution $p(\{\theta_j, \phi_j\}, 0)$ (the index $m = 1, \dots, M$ enumerates the different realizations). Then we propagate every initial vector $(\theta_0^{(m)}, \dots, \theta_N^{(m)}, \phi_0^{(m)}, \dots, \phi_N^{(m)})$ in time, so that after a lapse of time t , it evolves into a vector $(\Theta_0^{(m)}(t), \dots, \Theta_N^{(m)}(t), \Phi_0^{(m)}(t), \dots, \Phi_N^{(m)}(t))$. If the EOM 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: $x = \frac{1}{M} \times \sum_{m=1}^M \sin\Theta_j^{(m)} \bigotimes_{j=0}^N \langle \Theta_j^{(m)}, \Phi_j^{(m)} | X | \Theta_j^{(m)}, \Phi_j^{(m)} \rangle$.

To implement this approach, we need to determine the EOM for $\Theta_j(t)$, $\Phi_j(t)$ which would produce a good approximation for $p(\{\theta_j, \phi_j\}, t)$. First, let us find the exact EOM for $p(\{\theta_j, \phi_j\}, t)$. For simplicity, let us study one term in the Hamiltonian (1); i.e., we consider two spins $1/2$ (the central spin and the k th bath spin) coupled by the isotropic Heisenberg interaction $\mathcal{H}_k = A_k \mathbf{S}_0 \mathbf{S}_k$. The most general form for the two-spin density matrix is $\rho = w_{00} \mathbf{1}_0 \mathbf{1}_k + w_{0\alpha} \mathbf{1}_0 \sigma_k^\alpha + w_{\beta 0} \sigma_0^\beta \mathbf{1}_k + w_{\lambda\nu} \sigma_0^\lambda \sigma_k^\nu$, where $\alpha = x, y, z$ (and similarly for other Greek indices), and σ_0^α and σ_k^β denote the Pauli matrices for the 0th and the k th spin, respectively. Here and below, we assume summation over the repeating indices. From von Neumann's equation $\dot{\rho}(t) = i[\rho(t), \mathcal{H}]$, we obtain $\dot{w}_{00}(t) = 0$ [which expresses that $\text{Tr}\rho(t) = 1$], and

$$\begin{aligned} \dot{w}_{0\gamma}(t) &= \frac{A_k}{2} \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), \\ \dot{w}_{\gamma 0}(t) &= -\frac{A_k}{2} \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), \\ \dot{w}_{\alpha\beta}(t) &= \frac{A_k}{2} \epsilon_{\alpha\beta\gamma} [w_{\gamma 0}(t) - w_{0\gamma}(t)], \end{aligned} \quad (6)$$

where $\epsilon_{\alpha\beta\gamma}$ is a completely antisymmetric unity tensor (permutation symbol). These EOM determine the dynamics of $p(\{\theta_0, \phi_0, \theta_k, \phi_k\}, t)$. From the P representation (4), it follows that $p(\{\theta_0, \phi_0, \theta_k, \phi_k\}, t) = p_{00}(t) + p_{0\alpha}(t)c_k^\alpha + p_{\beta 0}(t)c_0^\beta + p_{\lambda\nu}(t)c_0^\lambda c_k^\nu$, where $p_{00} = (1/4\pi^2)w_{00}$, $p_{0\alpha} = (3/4\pi^2)w_{0\alpha}$, $p_{\alpha 0} = (3/4\pi^2)w_{\alpha 0}$, and $p_{\alpha\beta} = (9/4\pi^2)w_{\alpha\beta}$. Here we used the shorthand notations $c_0^\alpha = \sin\theta_0 \cos\phi_0$, $c_0^\beta = \sin\theta_0 \sin\phi_0$, $c_0^\gamma = \cos\theta_0$ (and similarly for $c_k^\alpha, c_k^\beta, c_k^\gamma$). The spherical harmonics of the order two and higher in $p(\{\theta_0, \phi_0, \theta_k, \phi_k\})$ are irrelevant: They do not change the density matrix [16].

The P representation for the many-spin density matrix (4) has a mean-field form; i.e., it is a product of single-spin density matrices $|\mu_j\rangle\langle\mu_j|$. This 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). However, the local fields should be redefined to provide an optimal approximation for $\mathbf{s}_0(t)$. For simplicity, we omit the discussion of the general form for $\mathbf{h}_0(t)$ and $\mathbf{h}_k(t)$ and proceed to the answer. We introduce the shorthand notations $C_0^x = \sin\Theta_0 \cos\Phi_0$, $C_0^y = \sin\Theta_0 \sin\Phi_0$, $C_0^z = \cos\Theta_0$ (and similarly for C_k^x, C_k^y, C_k^z) and postulate the following EOM:

$$\dot{\mathbf{C}}_0 = g_1[\mathbf{C}_k \times \mathbf{C}_0], \quad \dot{\mathbf{C}}_k = -g_2[\mathbf{C}_k \times \mathbf{C}_0] \quad (7)$$

[cf. Eq. (2)], where g_1 and g_2 are to be determined. By substituting these equations into the probability distribution $p(\{\Theta_0(t), \Phi_0(t), \Theta_k(t), \Phi_k(t)\}) = P_{00} + P_{0\alpha}C_k^\alpha + P_{\beta 0}C_0^\beta + P_{\lambda\nu}C_0^\lambda C_k^\nu$, and using the P representation (4), we obtain the following EOM for the density matrix ρ :

$$\begin{aligned} \dot{w}_{0\gamma}(t) &= -g_2 \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), & \dot{w}_{\gamma 0}(t) &= g_1 \epsilon_{\alpha\beta\gamma} w_{\alpha\beta}(t), \\ \dot{w}_{\alpha\beta}(t) &= (1/3) \epsilon_{\alpha\beta\gamma} [g_2 w_{0\gamma}(t) - g_1 w_{\gamma 0}(t)], \end{aligned} \quad (8)$$

[cf. Eqs. (6)], and $\dot{w}_{00}(t) = 0$. Equations (6) and (8) are incompatible; i.e., TDMF is never exact. However, we are interested only in $w_{\gamma 0}(t)$, since only this term determines the value of $\mathbf{s}_0(t)$. Therefore, we choose $g_1 = g_2 = g = A_k \sqrt{3}/2$ and differentiate Eqs. (6) and (8) with respect to time once more. Then both Eqs. (6) and (8) produce the same result: $\ddot{w}_{\gamma 0}(t) = -\ddot{w}_{0\gamma}(t) = (A_k^2/2)(w_{0\gamma} - w_{\gamma 0})$. Thus, the functions $w_{\gamma 0}(t)$ produced by the approximate Eqs. (7) and by the exact Eqs. (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. For polarized baths, one can use the perturbational approaches [8,9], so this limitation is not serious. Therefore, in order to fix the standard TDMF in the case of spins 1/2, we just need to replace A_k by $A_k \sqrt{3}/2$ in Eqs. (3). It may seem that we just derived the standard semiclassical EOM, 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 $g_1 = A_k \sqrt{3}/2$, $g_2 = A_k \sqrt{2}$. Moreover, the initial conditions in our approach and in the semiclassical approximation are different. For example, if the central spin 1/2 is initially directed along the z axis, then the initial density matrix $\rho(0) = 2^{-N} |\uparrow\rangle\langle\uparrow| \otimes_{k=1}^N \mathbf{1}$, and our approach requires $p(\{\theta_j, \phi_j\}, 0) = (4\pi)^{-N-1} (1 + 3 \cos\theta_0)$, while the semiclassics would correspond to $p(\{\theta_j, \phi_j\}, 0) = (4\pi)^{-N-1} \delta(\cos\theta_0 - 1)$, where $\delta(\dots)$ is the Dirac delta function.

The approach developed above gives excellent results at both short and long times, for different distributions of the couplings A_k , for various fields H_0 , for both longitudinal

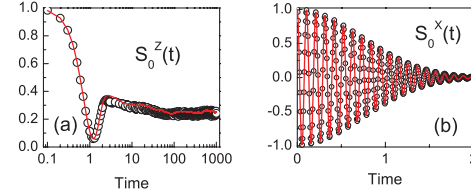


FIG. 1 (color). (a) Longitudinal $s_0^z(t)$ and (b) transverse $s_0^x(t)$ relaxation of the central spin 1/2 coupled to a bath of $N = 21$ spins 1/2. Couplings A_k are randomly distributed between 0 and 1.0, external fields are (a) $H_0 = 0$ and (b) $H_0 = 60.0$. Solid lines—exact solutions, open circles—approximation. Agreement is excellent.

and transverse relaxation, and for mixed initial state of the central spin. A small fraction of the representative tests for a moderate number of bath spins ($N = 15-20$) is shown in Figs. 1 and 2, where we used the Chebyshev expansion method [15] for exact solutions. The longitudinal decay shown in Fig. 1 is typical; the long-time tail suggests the slow relaxation $s_0^z(t) \sim 1/\ln t$, but the results are not conclusive, since for moderate-sized systems $s_0^z(t \rightarrow \infty)$ saturates at a value far from zero. We have to study much larger systems, where exact simulations are not possible due to exponential increase in computation time, and to use the approximate method.

We considered systems with $N = 1000-16000$ spins. For small $N = 2-5$, our approximation is very crude because the EOM (7) leads to the appearance of higher-order spherical harmonics in the function $p(\{\theta_j, \phi_j\}, t)$ (the terms proportional to $c_0^\alpha c_0^\beta c_k^\lambda c_k^\nu$, etc.). These terms do not change $\rho(t)$ [they disappear after integration in Eq. (4)], but they affect the EOM for physically relevant terms; i.e., the actual EOM for $w_{\gamma 0}(t)$ becomes $\ddot{w}_{\gamma 0}(t) = (A_k^2/2)(w_{0\gamma} - w_{\gamma 0}) + V$, where V is the contribution from the higher-order harmonics. However, the contribution of V into $\mathbf{s}_0(t)$ is bounded and quickly decreases for larger N , so we expect our approximation for $\mathbf{s}_0(t)$ to work better the larger N is. This is natural, since our method is based on TDMF, which works better for larger number of bath spins coupled to the central spin. Moreover, this assumption is well-confirmed by numerical tests. In Fig. 3, we present the

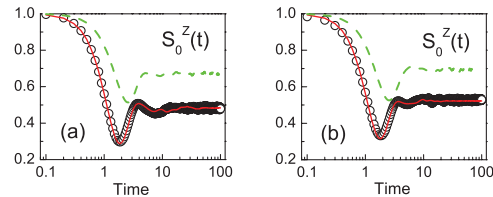


FIG. 2 (color). Longitudinal relaxation $s_0^z(t)$ of the central spin, couplings A_k are randomly distributed between -0.4 and 0.6 , field $H_0 = 1.0$. (a) Central spin 1/2, $N = 21$ bath spins; (b) central spin 1, $N = 19$ bath spins. Solid lines—exact solutions, open circles—our approximation; agreement is excellent. Dashed lines—standard TDMF; the disagreement with the exact solution is significant.

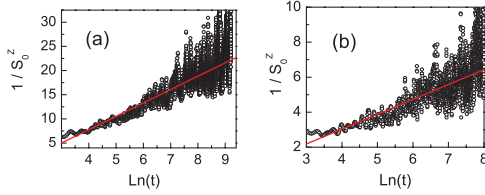


FIG. 3 (color). Long-time relaxation of the central spin $1/2$ coupled to a bath of 16000 spins $1/2$, field $H_0 = 0$. Graphs show $1/s_0^z(t)$ as a function of $\ln t$. The coupling constants were calculated as $A_k = (1/14)u(\mathbf{x}_k)$, where $u(\mathbf{x})$ is the electron density. (a) $u(\mathbf{x})$ 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) $u(\mathbf{x})$ is taken as an exponential function of \mathbf{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.

long-time longitudinal relaxation of an electron spin in a model quantum dot; we assumed that the bath spins $1/2$ are placed at the sites of a piece of a cubic lattice with the size $N_x \times N_y \times N_z$ ($N_x = N_y = 40$, $N_z = 10$, so the total number of bath spins $N = N_x N_y N_z = 16000$). The long-time relaxation clearly demonstrates that $s_0^z(t) \sim 1/\ln t$ (see [17]). Our studies show that the $1/\ln t$ decay 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. 3).

Our approach also performs well (see Fig. 4) 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 experiments of Ref. [2]. Figure 4(b) shows good qualitative agreement with the experimental curves [2], but the experiments are performed with $\sim 5\%$ – 10% bath polarization, and further development is needed for quantitative analysis.

Summarizing, we used the spin-coherent states P representation to develop a novel approach to the quantum central spin problem. 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

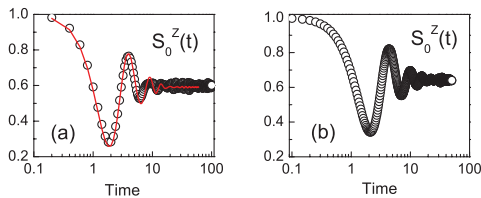


FIG. 4 (color). Longitudinal relaxation $s_0^z(t)$ of the central spin $1/2$ coupled to a bath of spins $1/2$ via the anisotropic X - Y Hamiltonian, external field $H_0 = 1.0$. (a) $N = 21$ bath spin, A_k are randomly distributed between 0 and 1.0. Solid line—exact solution, open circles—approximation.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

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] Note that $\tilde{A}(\theta, \phi) \neq \langle \theta, \phi | A | \theta, \phi \rangle$. Moreover, $\tilde{A}(\theta, \phi)$ is not unique: Any linear combination of spherical harmonics $Y_l^m(\theta, \phi)$ of the order $l > 2J$ can be added to it, without changing the operator A .
- [17] Similar relaxation was found in Ref. [12] for 2D Gaussian electron density, using adiabatic approximation applied to the semiclassical EOM. Accuracy of this method is unclear; it is supposed to be correct for large N , but we cannot confirm or reject that: For $N = 22$ the exact solution disagrees with the approximation of Ref. [12], and for larger N the exact solution is extremely difficult. Also, $1/\ln t$ was predicted from the perturbation theory for *polarized* baths [8] in the case of a 2D 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.