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Entanglement Dynamics of Two Qubits in a Common Bath

Jian Ma\(^1, 2\), Zhe Sun\(^1, 3\), Xiaoguang Wang\(^1, 2\), Franco Nori\(^1, 4\)

\(^1\)Advanced Science Institute, RIKEN, Wako-shi, Saitama 351-0198, Japan
\(^2\)Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University, Hangzhou 310027, China
\(^3\)Department of Physics, Hangzhou Normal University, Hangzhou 310027, China
\(^4\)Physics Department, The University of Michigan, Ann Arbor, MI 48109-1040, USA

We derive a set of hierarchical equations for qubits interacting with a Lorentz-broadened cavity mode at zero temperature, without using the rotating-wave, Born, and Markovian approximations. We use this exact method to reexamine the entanglement dynamics of two qubits interacting with a common bath, which was previously solved only under the rotating-wave and single-excitation approximations. With the exact hierarchy equation method used here, double excitations due to counter-rotating-wave terms are found to have remarkable effects on the dynamics and the steady state entanglement.

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I. INTRODUCTION

Decoherence is one of the most important problem in quantum information processing [1]. The description of this difficult problem usually involves various approximations. During the dynamic evolution, the system and the bath are mixed, and a perturbative treatment is required such that we can trace out the degrees of freedom of the bath. This perturbation is known as the Born approximation. Moreover, if the time scale of the bath is much shorter than that of the system, the Markovian approximation is often applied.

An effective method that avoids the above two approximations was developed by Tanimura et al. [2-4], who established a set of hierarchical equations [4] that includes all orders of system-bath interactions. The derivation of the hierarchy equations requires that the time-correlation function of the bath can be decomposed into a set of exponential functions [4]. At finite temperature, this requirement is fulfilled if the system-bath coupling can be described by a Drude spectrum. The hierarchy equation method is successfully used in describing quantum dynamics of chemical and biophysical systems [3-6], such as the light-harvesting complexes [6], of which the temperature of the environment is high enough, and the coupling between the system and the environment is too strong to enable a Born approximation. However, the powerful hierarchy equation method was seldom used in studying decoherence effects in quantum information [7]. Firstly, the operating temperature of qubit devices is very low. If we use the Drude spectrum, a numerical difficulty arises since the time-correlation function of the bath should be decomposed into a very large set of exponential functions [3]. Actually, the temperature of qubit devices is low enough that we can use a zero-temperature environment to model the decoherence. Secondly, the Drude spectrum is not quite general in qubit devices, especially when the qubit is placed in a cavity, and its environment is usually modeled by a Lorentz-broadened cavity mode.

In this paper we find that the hierarchy equation can also be derived at zero-temperature if we employ a Lorentz-type system-bath coupling spectrum. The set of hierarchy equations derived here provides an exact treatment of decoherence, and employs neither the rotating-wave, Born, nor Markovian approximations. System-bath correlations are here fully accounted during the entire time evolution, as compared to traditional master equation treatments, the correlations are truncated to second order. High-order correlations are shown [8] to be very important, even producing a totally different physics. Moreover, the hierarchy equation we derive here is found to be effective in the single-mode case, and is a promising method for studying strong- and ultrastrong-coupling physics [7, 9].

We use the hierarchy equation method to study a model of two qubits interacting with a common bosonic bath, which is widely considered in studying decoherence-free subspace [10] and bipartite entanglement dynamics [11]. This model was solved exactly [1, 12] under the rotating-wave approximation (RWA). It is not surprising that entanglement can be generated for a separable initial state, since the bath induces an effective qubit-qubit interaction. Another observation based on the RWA lies in the steady-state entanglement, which is determined only by the overlap between the initial state and the decoherence-free state, independent of the system-bath coupling [12]. This is because the dynamics of the qubit is restricted to a single-excitation subspace. However, when the counter-rotating terms are accounted, double excitation occurs and the steady-state entanglement vanishes for certain system-bath couplings. We will demonstrate this observation below.

II. HIERARCHY EQUATION METHOD

Here we first consider qubits interacting with a bosonic bath, also known as the spin-boson model:

\[ H = H_S + H_B + H_{\text{Int}}, \] (1)
where \( H_S \) is the free Hamiltonian of the qubit and (with \( \hbar = 1 \))

\[
H_B = \sum_k \omega_k b_k^\dagger b_k, \\
H_{\text{Int}} = \sum_k V \left( g_k b_k + g_k^* b_k^\dagger \right),
\]

(2)

if the qubit and bath are initially in a separable state, i.e., \( \rho(0) = \rho_S(0) \otimes \rho_B \), where \( \rho_B = \exp(-\beta H_B)/Z_B \) is the initial state of the bath, with \( \beta = 1/T \) (with \( k_B = 1 \)) and \( Z_B \) is the partition function. In Eq. (3), \( T \) is the chronological time-ordering operator, which orders the operators inside the integral such that the time arguments increase from right to left. Two superoperators are introduced, \( A^\gamma B \equiv [A, B] = AB - BA \) and \( A^\circ B \equiv \{A, B\} = AB + BA \). Also, \( C^R (t_2 - t_1) \) and \( C^I (t_2 - t_1) \) are the real and imaginary parts of the bath time-correlation function

\[
C(t_2 - t_1) \equiv \langle B(t_2) B (t_1) \rangle = \text{Tr} [B(t_2) B (t_1) \rho_B],
\]

(4)

respectively, and

\[
B(t) = \sum_k \left( g_k b_k e^{-i\omega_k t} + g_k^* b_k^\dagger e^{i\omega_k t} \right).
\]

(5)

Equation (3) is difficult to solve directly, due to the time-ordered integral. An effective method for this problem was developed \([2-5]\) by solving a set of hierarchy equations, such as the form of Eq. (9). The hierarchy equations are obtained by repeatedly taking the derivative of the right-hand side when the system-bath coupling is described by the Drude spectrum \( J(\omega) = \frac{\lambda}{\pi} \frac{1}{(\omega - \omega_0)^2 + \gamma^2} \) at finite temperatures, where \( \eta \) is the reorganization energy, and \( \omega_c \) is the decay rate of the bath correlation function. A key condition in deriving the hierarchy equation is that, with the Drude spectrum, the correlation function (5) can be decomposed into a sum of exponential functions of time as \( C(t_2 - t_1) = \sum_k f_k \exp(-\gamma_k) \), where \( \gamma_k = \frac{\lambda}{2\omega_c} (1 - \delta_{k,0}) + \omega_c \delta_{k,0} \) are the Matsubara frequencies. The hierarchy equation method enables a rigorous study of decoherence-related effects in chemical physics and biophysics \([6]\). In such systems, the coupling strength between the system and bath is not always weak, and the temperature \( T \) is so high that only a few Matsubara terms could provide enough numerical precision \([3]\). However, the number of Matsubara terms in the expansion increases with decreasing temperature, which is difficult to handle numerically. This problem becomes serious when we consider qubit devices, which are generally prepared in nearly zero-temperature environments, and thus prevent the use of the original hierarchy equation method. Fortunately, the exponential decay of bath correlation functions at zero temperature occurs in many quantum computing devices, such as cavity-qubit systems, where the coupling spectrum between the qubits and cavity modes is usually Lorentz type, but not Drude type, so in that case the hierarchy method can also be applied.

Now we consider qubits interacting with a single mode of the cavity, with frequency \( \omega_0 \). Due to the imperfection of the cavity, the single mode is broadened and the qubit-cavity coupling spectrum becomes Lorentz-type

\[
J(\omega) = \frac{\lambda}{\pi} \frac{1}{(\omega - \omega_0)^2 + \gamma^2},
\]

(6)

where \( \lambda \) reflects the system-bath coupling strength, \( \gamma \) is the broadening width of the cavity mode, and \( \tau_c = 1/\gamma \) is the lifetime of the mode. At \( T = 0 \), if the cavity is initially in a vacuum state \( \otimes \kets{0}_g \), the time-correlation function (5) becomes

\[
C(t_2 - t_1) = \lambda \exp\left[ -\left( \gamma + i\omega_0 \right)|t_2 - t_1| \right],
\]

(7)

which is an exponential form that we need to use for the hierarchy equations. In the single-mode limit, \( \gamma = 0 \) and \( C(t_2 - t_1) = \lambda \exp\left[ -i\omega_0 |t_2 - t_1| \right] \), and we see that \( \lambda \) is related to the square of the Rabi oscillation frequency.

To derive the hierarchy equation in a convenient form, we further write the real and imaginary parts of the time-correlation function (7) as

\[
C^R(t) = \sum_{k=1}^{\infty} \frac{\lambda}{2} e^{-\nu_k t}, \quad C^I(t) = \sum_{k=1}^{\infty} \frac{(-1)^k}{2} \lambda e^{-\nu_k t},
\]

(8)

where \( \nu_k = \gamma + (-1)^k i\omega_0 \). Then, following procedures shown in Appendix A and Ref. \([2, 4]\), the hierarchy equations of the qubits are obtained

\[
\frac{\partial}{\partial t} \varphi(t) = -iH_S^x + \vec{n} \cdot \vec{\sigma} \varphi(t) - \frac{1}{2} \sum_{k=1}^{\infty} V^x \varphi_{\vec{\sigma} + \vec{e}_k}(t) - \frac{i}{2} \sum_{k=1}^{\infty} n_k \left[ V^x + (-1)^k V^o \right] \varphi_{\vec{\sigma} - \vec{e}_k}(t),
\]

(9)
where the subscript \( \vec{n} = (n_1, n_2) \) is a two-dimensional index, with \( n_1(2) \geq 0 \), and \( \rho_\vec{n}(t) \equiv \varrho_{\vec{n},0,0}(t) \). The vectors \( \vec{c}_1 = (1, 0) \), \( \vec{c}_2 = (0, 1) \), and \( \vec{v} = (\nu_1, \nu_2) = (\gamma - i\omega_0, \gamma + i\omega_0) \). We emphasize that \( \varrho_{\vec{n}}(t) \) with \( \vec{n} \neq (0, 0) \) are auxiliary operators introduced only for the sake of computing, they are not density matrices, and are all set to be zero at \( t = 0 \). The hierarchy equations are a set of linear differential equations, and can be solved by using the Runge-Kutta method. The contributions of the bath to the dynamics of the system, including both dissipation and Lamb shift, are fully contained in the hierarchy equation (9). The Lamb shift term [13], which is related to the imaginary part of the bath correlation function, can be written explicitly in the common non-Markovian equations. Since the real and imaginary parts of the bath correlation function are taken into considered here, the effects of the Lamb shift exist in the hierarchy equations, although not in an explicit form.

For numerical computations, the hierarchy equation (9) must be truncated for large enough \( \vec{n} \). We can increase the hierarchy order \( \vec{n} \) until the results of \( \rho_\vec{n}(t) \) converge. The terminator of the hierarchy equation is

\[
\frac{\partial}{\partial t} \varrho_{\vec{n}}(t) = -\left(iH_{\vec{n}}^\varsigma + \vec{N} \cdot \vec{v}\right) \varrho_{\vec{n}}(t) - \frac{\Lambda}{2} \sum_{k=1}^{2} n_k \left[V^x + (-1)^k V^o\right] \varrho_{\vec{n} - \vec{c}_k}(t),
\]

(10)

where we dropped the deeper auxiliary operators \( \varrho_{\vec{n} + \vec{c}_k} \).

The numerical results in this paper were all tested and converged, and the density matrix \( \rho_\vec{n}(t) \) is positive.

### III. ENTANGLEMENT OF TWO QUBITS IN A COMMON BATH

Below we apply the hierarchy equation (9) to a widely studied model: two qubits interacting with a common bath. The model is used to study decoherence-free space [10], bath induced entanglement [12], and other related topics [11]. In previous works [12, 14, 15], the RWA was used, and the exact dynamics could only be found in a single-excitation subspace. Without using the RWA, the model was also studied [21–23] in a perturbative way. However, if the system-bath coupling becomes strong enough, which is explored in recent experiments [9], both the RWA and perturbation methods fail. Therefore the hierarchy method is very suitable in such conditions.

Consider two qubits interacting with a common bosonic bath. The system Hamiltonian in Eq. (1) is now given by

\[
H_S = \frac{\omega_1}{2}\sigma_{1z} + \frac{\omega_2}{2}\sigma_{2z},
\]

(11)

and below we consider \( \omega_1 = \omega_2 = \omega_0 \), i.e., the resonant case. The system operator in Eq. (2) is set by \( V = \alpha_1\sigma_{1x} + \alpha_2\sigma_{2x} \), and for simplicity, we consider \( \alpha_1 = \alpha_2 =

![Figure 1: (Color online) Concurrence versus time for the initial state \( |\psi(0)\rangle = |0\rangle_1|0\rangle_2 \) with different values of \( \gamma \). Here \( \lambda = 0.1\omega_0 \) is in the strong-coupling regime. In the single-mode limit, \( \gamma = 0 \), the result of the hierarchy equation (solid) coincides with direct numerical calculations (circles). The entanglement suddenly vanishes and revivals are observed. When increasing \( \gamma \), the oscillations and the maximum entanglement are suppressed. Under the RWA, the initial state does not evolve, and the entanglement stays at zero.](image)

1. This model is exactly solvable [12] when the RWA is applied and the initial state is of the form

\[
|\psi(0)\rangle = |c_1(0)|1\rangle_1|0\rangle_2 + |c_2(0)|0\rangle_1|1\rangle_2 \otimes |0_k\rangle.
\]

(12)

The time evolution is then given by

\[
|\psi(t)\rangle = |c_1(t)|1\rangle_1|0\rangle_2 + |c_2(t)|0\rangle_1|1\rangle_2 \otimes |0_k\rangle + \sum_k c_k(t) |0\rangle_1|0\rangle_2|1_k\rangle,
\]

(13)

where \( |1_k\rangle \) denotes that only the \( k \)th mode of the bath is excited. The explicit forms of \( c_1(t) \) and \( c_2(t) \) are given in Ref. [12]. The time evolution of the density matrix is

\[
\rho(t) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & |c_1(t)|^2 & c_1(t)c_2^*(t) & 0 \\
0 & c_2(t)c_1^*(t) & |c_2(t)|^2 & 0 \\
0 & 0 & 0 & 1 - |c_1(t)|^2 - |c_2(t)|^2
\end{pmatrix},
\]

(14)

which is obviously restricted to a single-excitation space, and thus the concurrence of the above density matrix is

\[
C(t) = 2|c_1(t)c_2^*(t)|.
\]

(15)

We first compare the above results with our hierarchy method for the initial state \( |\psi(0)\rangle = |0\rangle_1|0\rangle_2 \), shown in Fig. 1. The system-bath coupling is set by \( \lambda = 0.1\omega_0 \), which already enters the strong-coupling regime. Such an initial state does not evolve under the RWA, and then
steady-state entanglement is shown in (d), and it vanishes if no entanglement will be produced. However, from Fig. 1 we observe the generation of considerable entanglement, even with large $\gamma$. The RWA fails in predicting the real physics. Since the coupling is strong, the oscillation for small $\gamma$ case is drastic. The sudden vanishing and revival of entanglement were observed, and with increasing of $\gamma$, the oscillations of the concurrence were suppressed. It should be emphasized that, when $\gamma = 0$, the results obtained by the hierarchy equations coincide with our exact numerical results obtained by solving the single-mode Hamiltonian directly. Therefore, by using a unified method, we can study the dynamics of the system interacting with a bath from the single-mode to multimode regime.

Another interesting result here is about the steady-state entanglement. Under the RWA, the dynamics is in the single-excitation subspace, only two states are independent, $|\varphi_{\pm}\rangle = (|0\rangle_1|1\rangle_2 \pm |1\rangle_1|0\rangle_2)/\sqrt{2}$. The state $|\varphi_{-}\rangle$ is decoherence-free; this means that if the initial state has non-vanishing overlap with $|\varphi_{-}\rangle$, the steady state is entangled, and the concurrence becomes

$$C (t \to \infty) = C (|\varphi_{-}\rangle \langle \varphi_{-} |\psi (0)\rangle)^2 = |\langle \varphi_{-} |\psi (0)\rangle|^2,$$

which is independent of the system-bath coupling strength $\lambda$ and the bath-decay rate $\gamma$. However, if $\lambda$ is not very small, although $|\varphi_{-}\rangle$ is also decoherence-free, Eq. (16) should be reexamined by using a more rigorous treatment, since double excitations need to be accounted. Actually, the reliability of the RWA was discussed in many literatures [16–24]. As shown in Refs. [16, 24], counter-rotating-wave terms can induced a significant shift in the population of the steady state even in the bad-cavity case.

In Fig. 2, we show the results given by the hierarchy method. The initial state there is $|\psi (0)\rangle = (2|0\rangle_1|1\rangle_2 + |1\rangle_1|0\rangle_2)/\sqrt{5}$. According to Eq. (16), the concurrence of the steady state is $0.1$. We can see in Fig. 2(a)-(c) that increasing $\gamma$ the concurrence of the steady state decreases. In Fig. 2(d), we show that for a given $\lambda = 0.01\omega_0$, the steady-state entanglement vanishes when $\gamma$ is larger than a critical value. This reflects the importance of the counter-rotating-wave terms, which break the single-excitation condition and give a totally different steady-state entanglement. Similar results are obtained in Ref. [24], where the increase of the cavity decay rate is found to decrease the maximum of induced entanglement, and the steady state that computed without RWA has no entanglement but finite discord. This simple example indicates that some exact results previously obtained under the RWA need to be reexamined.

IV. CONCLUSION

In summary, we derive a set of hierarchy equations at zero temperature with a Lorentz spectrum. This set of equations is very suitable for qubit-cavity systems, especially when the interaction is so strong that the RWA and perturbative methods break down. It even works well when the bath has only one single mode. Moreover, this equation is very flexible. For example, if the qubits interact with several cavity modes, each broadened into a Lorentz form, then the bath correlation functions can also be expanded as several exponential functions. Thus the form of the hierarchy equations remains. The hierarchy equations are applied to reexamine the dynamics of two qubits interacting with a common bath. Previous works usually employed the RWA, and the results were restricted to the single-excitation space. This is not the case in this paper, since we do not use the RWA, and the counter-rotating-wave terms will cause double-excitations. We found that the steady-state entanglement depends on the system-bath coupling spectrum. For a given coupling strength $\lambda$, there will be no steady state entanglement when $\gamma$ is larger than a critical value. The exact dynamics exhibits a totally different physics, compared to the RWA model, which motivates the reexamination of many previous approximate studies.

V. ACKNOWLEDGEMENTS

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which is a direct result of Eq. (5). The idea of the hierarchy equation method [2, 4] is to transform such an integral equation to a group of ordinary differential equations. The derivation of the hierarchy equations is straightforward: taking the time derivative of Eq. (A1) repeatedly.

We first take the time derivative of Eq. (A1) and obtain

$$\frac{\partial}{\partial t} \rho_S (t) = -i H^\times \rho_S (t) + \Phi \sum_{k=1}^2 F_k (t), \quad (A3)$$

where

$$F_k (t) = U (t) T \left\{ \int_0^t d\tau e^{-i k (t-\tau)} \Theta_k (\tau) \exp \left[ \int_0^t d\tau_1 \int_0^{t_2} dt_1 \Phi (t_2) \sum_{n=1}^2 e^{i \nu_n (t_2-\tau_1)} \Theta_n (\tau_1) \right] \rho_S (0) U (t)^\dagger \right\}. \quad (A4)$$

Thus the solution of $\rho_S (t)$ is determined by (i) its own free evolution, (ii) the dynamics of $F_k (t)$. The initial condition of $F_k (t)$ is

$$F_k (0) = 0, \quad (A5)$$

which is a direct result of Eq. (A4). To solve for $F_k (t)$, we need its differential equation. Before taking the time derivative of $F_k (t)$, we first introduce the following useful notations [4]:

$$\varrho (0, 0) (t) \equiv \rho_S (t),$$
$$\varrho (1, 0) (t) \equiv \varphi_1 (t),$$
$$\varrho (1, 1) (t) \equiv \varphi_2 (t). \quad (A6)$$

Then Eq. (A3) can be rewritten as

$$\frac{\partial}{\partial t} \rho_S (t) = -i H^\times \rho_S (t) + \Phi \sum_{k=1}^2 \varrho_k (t) + \tilde{c}_k \rho_S (t), \quad (A7)$$

where $\tilde{c}_1 = (1, 0)$ and $\tilde{c}_2 = (0, 1)$.

The differential equations of $\varrho (1, 0) (t)$ and $\varrho (1, 1) (t)$ are obtained as
\[
\begin{align*}
\frac{\partial}{\partial t} \varrho_{(1,0)} (t) &= - (iH_S^x + \nu_1) \varrho_{(1,0)} (t) + \Phi \sum_{k=1}^{2} \varrho_{(1,k)} (t) + \Theta_1 \varrho_{(0,0)} (t) \\
\frac{\partial}{\partial t} \varrho_{(0,1)} (t) &= - (iH_S^x + \nu_2) \varrho_{(0,1)} (t) + \Phi \sum_{k=1}^{2} \varrho_{(0,k)} (t) + \Theta_2 \varrho_{(0,0)} (t),
\end{align*}
\]

where we find three new auxiliary matrices,

\[
\begin{align*}
\varrho_{(2,0)} (t) &= U (t) \left\{ \left[ \int_0^t d\tau e^{-\nu_1 (t-\tau)} \Theta_1 (\tau) \right]^2 \right. \\
& \left. \times \exp \left[ \int_0^t dt_2 \int_0^{t_2} dt_1 \Phi (t_2) \sum_{k=1}^{2} e^{\nu_k (t_2-t_1)} \Theta_k (t_1) \right] \right\} \rho_S (0) U (t) ,
\end{align*}
\]

\[
\begin{align*}
\varrho_{(1,1)} (t) &= U (t) \left\{ \left[ \int_0^t d\tau e^{-\nu_1 (t-\tau)} \Theta_1 (\tau) \right] \left[ \int_0^t d\tau e^{-\nu_2 (t-\tau)} \Theta_2 (\tau) \right] \right. \\
& \left. \times \exp \left[ \int_0^t dt_2 \int_0^{t_2} dt_1 \Phi (t_2) \sum_{k=1}^{2} e^{\nu_k (t_2-t_1)} \Theta_k (t_1) \right] \right\} \rho_S (0) U (t) ,
\end{align*}
\]

\[
\begin{align*}
\varrho_{(0,2)} (t) &= U (t) \left\{ \left[ \int_0^t d\tau e^{-\nu_2 (t-\tau)} \Theta_2 (\tau) \right]^2 \right. \\
& \left. \times \exp \left[ \int_0^t dt_2 \int_0^{t_2} dt_1 \Phi (t_2) \sum_{k=1}^{2} e^{\nu_k (t_2-t_1)} \Theta_k (t_1) \right] \right\} \rho_S (0) U (t) .
\end{align*}
\]

By repeating the above procedures, we find

\[
\frac{\partial}{\partial t} \varrho_{\vec{n}} (t) = - (iH_S^x + \vec{n} \cdot \vec{\nu}) \varrho_{\vec{n}} (t) + \Phi \sum_{k=1}^{2} \varrho_{\vec{n}+\vec{e}_k} (t) + \sum_{k=1}^{2} n_k \Theta_k \varrho_{\vec{n}-\vec{e}_k} (t),
\]

where \(\vec{n} = (n_1, n_2)\) is a two-dimensional index, with \(n_1(2) \geq 0\). The two-dimensional vector \(\vec{\nu} = (\nu_1, \nu_2) = (\gamma - i\omega_0, \gamma + i\omega_0)\). The auxiliary matrix is

\[
\begin{align*}
\varrho_{\vec{n}} (t) &= U (t) \left\{ \left[ \int_0^t d\tau e^{-\nu_1 (t-\tau)} \Theta_1 (\tau) \right]^{n_1} \left[ \int_0^t d\tau e^{-\nu_2 (t-\tau)} \Theta_2 (\tau) \right]^{n_2} \right. \\
& \left. \times \exp \left[ \int_0^t dt_2 \int_0^{t_2} dt_1 \Phi (t_2) \sum_{k=1}^{2} e^{\nu_k (t_2-t_1)} \Theta_k (t_1) \right] \right\} \rho_S (0) U (t) .
\end{align*}
\]

Inserting Eq. (A2) into Eq. (A12), we obtain the explicit form of the hierarchy equation as

\[
\begin{align*}
\frac{\partial}{\partial t} \varrho_{\vec{n}} (t) &= - (iH_S^x + \vec{n} \cdot \vec{\nu}) \varrho_{\vec{n}} (t) \\
& - i \sum_{k=1}^{2} V^x \varrho_{\vec{n}+\vec{e}_k} (t) \\
& - i \sum_{k=1}^{2} \frac{n_k}{2} \left[ V^x + (-1)^k V^o \right] \varrho_{\vec{n}-\vec{e}_k} (t).
\end{align*}
\]

The initial conditions are

\[
\varrho_{\vec{n}} (0) = \begin{cases} 
\rho_S (0), & \text{for } n_1 = n_2 = 0, \\
0, & \text{for } n_1 > 0, \ n_2 > 0.
\end{cases}
\]

Although the explicit form of \(\varrho_{\vec{n}} (t)\) is complicated, we need only to focus on its differential equations, which can be solved directly by using the traditional Runge-Kutta method.


