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TWO INTERACTING SPINS IN EXTERNAL FIELDS AND APPLICATION TO QUANTUM COMPUTATION

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We study the four-level system given by two quantum dots immersed in a time-dependent magnetic field, which are coupled to each other by an effective Heisenberg-type interaction. We describe the construction of the corresponding evolution operator in a special case of different time-dependent parallel external magnetic fields. We find a relation between the external field and the effective interaction function. The obtained results are used to analyze the theoretical implementation of a universal quantum gate.

Изучается четырехуровневая система, отвечающая двум квантовым точкам с взаимодействием Гейзенберга, помещенным во внешнее зависящее от времени магнитное поле. Построен оператор эволюции для случая, когда магнитные поля в каждой точке параллельны. Указана связь между магнитными полями и эффективной функцией взаимодействия спинов. Обсуждается применение полученных результатов к построению универсального квантового ключа.

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INTRODUCTION

In quantum computers (QC) the classical bit is replaced by the states of a two-level quantum system, and the computation is performed by the manipulation of these systems. These two-level quantum systems are called *qubits* and these manipulations — *quantum gates*. As for classical computers, for QC the accomplishment of an arbitrary algorithm can be performed using just a few specific manipulations called *universal quantum gates*. With these universal quantum gates, a process that acts in an arbitrary number of qubits can be constructed using gates that act only in one and two qubits. It is believed that, as for classical computers, for QC the most promising candidate for a possible large-scale implementation is solid-state devices. Among these devices, one can highlight the system of two coupled semiconductor quantum dots (QD) [1]. In this system the qubits are the one-half spin states of

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an excess electron in each dot, and the universal quantum gates can be performed by applying external electromagnetic pulses to the dots.

In the present work we study the behavior of two coupled QD, when each dot is subject to different time-dependent parallel external magnetic fields, and discuss the use of this system to implement a universal quantum gate.

1. TWO COUPLED QUANTUM DOTS

The most general Hamiltonian $\hat{H}(\mathbf{G},\mathbf{F},J)$ of two interacting spin-$1/2$ particles, subject to the external fields $\mathbf{G}$ and $\mathbf{F}$, respectively, is (we set $\hbar = 1$)

$$\begin{gathered}\hat{H}(\mathbf{G},\mathbf{F},J) = (\boldsymbol{\rho}\cdot\mathbf{G}) + (\boldsymbol{\Sigma}\cdot\mathbf{F}) + J_{ij}\Theta^{ij}/2,\\ \boldsymbol{\rho} = \boldsymbol{\sigma}\otimes I,\ \boldsymbol{\Sigma} = I\otimes\boldsymbol{\sigma},\ \Theta^{ij} = \sigma_i\otimes\sigma_j,\end{gathered} \tag{1}$$

where J_{ij} are 9 independent functions of time; $\mathbf{G}$ and $\mathbf{F}$ are time-dependent three-vectors; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices and I is the 2×2 identity.

Note that the interaction with the external fields in (1) is given by the solutions of the *single-spin equation* (SSE) [5],

$$i\dot{\psi} = \hat{h}\psi, \quad \psi^T = (v_1, v_2), \quad \hat{h} = (\boldsymbol{\sigma}\cdot\mathbf{K}), \tag{2}$$

that describe a single fixed spin-$1/2$ particle immersed in an external field $\mathbf{K}(t)$.

The Hamiltonian (1) can be used to describe the coupling between two QD. When these QD are used to implement a quantum gate, the action of the gate corresponds to the variation of the external fields during a certain time τ. The matrices Θ^{ij} in (1) can be chosen spherically symmetric, $\Theta^{ij} \equiv \boldsymbol{\Sigma}\cdot\boldsymbol{\rho} = \Sigma_{i=1}^{3}\sigma_i\otimes\sigma_i$, if the system obeys the following conditions (see [1]):

1) the time τ cannot be too small, to avoid transitions to higher energy levels, so that the difference between energy levels ΔE should be larger than $\hbar/\tau$;

2) the decoherence time of the physical system should be much larger than τ.

Under these conditions, the Hamiltonian (1) becomes

$$\hat{H}(\mathbf{G},\mathbf{F},J) = (\boldsymbol{\rho}\cdot\mathbf{G}) + (\boldsymbol{\Sigma}\cdot\mathbf{F}) + \frac{J(\boldsymbol{\Sigma}\cdot\boldsymbol{\rho})}{2}. \tag{3}$$

The above interaction is known as the *Heisenberg interaction.* We call the Schrödinger equation with the Hamiltonian (3) *the two-spin equation* (TSE).

2. PARALLEL PULSES

The use of two coupled spin-$1/2$ particles to implement quantum algorithms requires the control of individual spins and an interaction capable of creating an entangled state starting from an original product state [2]. In a system described by the Hamiltonian (3) the individual spins are controlled by the fields $\mathbf{F}$ and $\mathbf{G}$ and, when these fields are zero ($\mathbf{F} = \mathbf{G} = \mathbf{0}$), the evolution operation $R_t(\mathbf{G},\mathbf{F},J)$ of the problem can be written as [3]

$$R_t(0,0,J) = \exp\left[\frac{i\Phi(t)}{2}\right]\left[\mathbb{I}\cos\Phi(t) - iA\sin\Phi(t)\right],$$
$$A = \frac{1}{2}\left[\mathbb{I} + (\mathbf{\Sigma}\cdot\boldsymbol{\rho})\right], \quad \Phi(t) = \int_{t_0}^{t} J(\tau)\, d\tau, \tag{4}$$

where $\mathbb{I}$ is the 4×4 unit matrix. The above expression shows that, for $\Phi = \pi/4$, the evolution operator acts as the gate known as square root of swap ($U_{\rm sw}^{1/2}$), that is capable of entangling an initial product state. With the $U_{\rm sw}^{1/2}$ we can construct the universal XOR gate as [4]

$$U_{\rm XOR} = \exp\left(\frac{i\pi\rho_3}{4}\right)\exp\left(-\frac{i\pi\Sigma_3}{4}\right)U_{\rm sw}^{1/2}\exp\left(\frac{i\pi\rho_3}{2}\right)U_{\rm sw}^{1/2}. \tag{5}$$

The above expression shows that we can construct any quantum gate by a sequence of pulses that turn the external fields and the interaction on and off. So, in principle, we do not need the exact solutions of the TSE, once we can describe this series of pulses using Eq. (4) and the solution of the SSE (2). However, the construction of gates by a sequence of pulses is not appropriate, because the duration of the entire sequence can be too long, violating the condition (2) of the preceding section, or the pulses need to vary too fast, violating the condition (1). So, it is important to implement the gates at once, applying just one adequate field, called the *parallel pulse* [4]. In the case of the XOR gate (5), in order to use a parallel pulse, one needs to find a field whose evolution operation, at a given instant τ of time, has the form

$$R_\tau(\mathbf{G},\mathbf{F},J) = U_{\rm XOR} = \exp\left[-\frac{i\pi(\Sigma_3\rho_3 + \Sigma_3 + \rho_3)}{4}\right]. \tag{6}$$

In order to find this parallel pulse, in a general case, we need to construct the evolution operator of the TSE for different kinds of external fields and interactions.

3. EVOLUTION OPERATOR OF THE TSE

In what follows we will work out problems where the external fields at the two spins have an arbitrary and independent time-dependence, but with the fields in the same direction (we choose the z direction),

$$\mathbf{G} = (0,0,B_1), \quad \mathbf{F} = (0,0,B_2), \quad B_{1,2} = B_{1,2}(t). \tag{7}$$

In this case, the Hamiltonian (3) assumes the form

$$\hat{H} = \frac{1}{2}\left[(\Sigma_3 + \rho_3)B_+ - (\Sigma_3 - \rho_3)B_- - J\right] + AJ, \quad B_\pm(t) = B_1(t) \pm B_2(t), \tag{8}$$

with the constant 4×4 orthogonal matrix A given in (4).

The evolution operator of the TSE with the Hamiltonian (8) can be written as [3]

$$R_t(\mathbf{G},\mathbf{F},J) = \exp\left(-\frac{i}{2}\left[(\Sigma_3+\rho_3)\,\Gamma(t)+\Sigma_3\rho_3\Phi(t)\right]\right)M(t),$$
$$\Gamma(t)=\int_0^t B_+(\tau)\,d\tau,\quad \Phi(t)=\int_0^t J(t)\,d\tau,\quad M=\begin{pmatrix}1&0&0\\0&\hat{u}_t&0\\0&0&1\end{pmatrix}, \tag{9}$$

where the 4×4 matrix $M\,(t)$ is given in terms of the 2×2 evolution operator $\hat{u}_t=\hat{u}_t\,(J,B_-)$ of the SSE (2) with the effective external field

$$\mathbf{K}\,(t) = (J\,(t)\,,0,B_-\,(t))\,. \tag{10}$$

Therefore, in this case, the TSE problem reduces to finding solutions of a SSE. In addition, although the obtained expressions depend on the sum and the difference between the fields at the spins, only the average value of this sum is relevant, so that the explicit form of its time variation can be arbitrary.

3.1. Exact Solutions of the Single-Spin Equation. To construct the evolution operator for the TSE (9) we need exact solutions of the SSE (2). A number of exact solutions of the SSE were found in [5, 6]. For periodic or quasiperiodic external fields, the SSE has been studied by many authors using different approximation methods, e.g., perturbative expansions [7].

The most complete description of the known exact solutions of the SSE can be found in our previous work [5]. In this work we present the exact solutions for 26 families of external fields in the form (10). For each of these solutions we show that a solution for a given $\mathbf{K}\,(J,B_-)$ produces the solution for $\mathbf{K}\,(B_-,J)$, so that we can interchange the role of the external fields' difference and the interaction function. Besides, in the cited article, we develop a method of constructing new exact solutions starting from a previously known solution, using the Darboux transformation. The solutions obtained in that way have a varied functional dependence (polynomial, trigonometric, hyperbolic, etc.), which gives a wide range of fields to choose from that are more appropriate to adjust to experimental setups.

3.2. The Interaction Function. The effective field $\mathbf{K}$ (10) shows that, in order to use the parallel field to implement a quantum gate, we need to vary independently the interaction and the fields' difference. Using the *Heitler–London* approximation it is possible to obtain an expression for the effective interaction function $J\,(a,B_1,B_2)$ as a function of the inter-dot distance (a), and the external magnetic field at each dot (B_1 and B_2). The detailed calculations can be found in our work [8], and the obtained expressions give

$$J=\frac{\left(1-\Delta^2\right)}{\left(2\sinh\left(2M\right)+\Delta\exp\left(-2M\right)\left(2-\Delta^3\right)\right)}\left[L-\frac{\hbar\omega_0}{4}\frac{\left(b_2^2-b_1^2\right)\left(b_1-b_2\right)}{b_2b_-}\right],$$
$$M=\frac{2\left(ea\right)^2}{a_0^2\left(b_2+b_1\right)}\left[\frac{b_1b_2}{e^2}+\left(\frac{B_2+B_1}{8mc\omega_0^2}\right)^2\right],\;b_i^2=1+\left(\frac{eB_i}{2mc\omega_0}\right)^2,\;\Delta=\frac{b_1-b_2}{b_1+b_2}, \tag{11}$$

where m is the effective mass of the electron in the dot [9], ω_0 is a characteristic parameter of the dot [10], $a_0 = \sqrt{\hbar / m\omega_0}$ is the effective Bohr radius, and

$$L = \frac{\hbar\omega_0}{2}\left\{\frac{3}{2d^2\left(b_- + b_+\right)^2}\left[\frac{1+\Delta^2}{\left(1-\Delta^2\right)^2} - 1\right] - 3\left(\frac{\Delta^2 - 1}{b_1 + b_2}\right) - \frac{d^2}{2}\left(\Delta^4 - 6\Delta^2 - 3\right)\right\} + \\ + \frac{e^2}{a_0\kappa}\sqrt{\frac{\pi}{2}}\bar{b}\left\{\sqrt{\left(1-\Delta^2\right)}\exp\left[-d^2\left(1-\Delta^2\right)\bar{b}\right]\mathrm{I}_0\left[d^2\left(1-\Delta^2\right)\bar{b}\right] - \right. \\ \left. - \exp\left(\frac{d^2}{2}K\right)\mathrm{I}_0\left(\frac{d^2}{2}K\right)\right\}, \quad (12)$$

$$K = \bar{b}\left(1+\Delta^2\right) - \frac{1}{\bar{b}} + \sqrt{\left[\left(1-\Delta^2\right)\bar{b}\right]^2 - 2\left(1+\Delta^2\right) + \frac{1}{\bar{b}^2}}, \ \bar{b} = \frac{b_1 + b_2}{2}, \ d = \frac{a}{a_0},$$

where I_0 is the zeroth-order Bessel function, e is the charge of electron, and κ is the dielectric constant of the medium. From the above expressions we see that

$$J\left(a, B_+, B_-\right) = J\left(a, B_+\right) + O\left(\Delta^2\right), \ \Delta = B_-/B_+.$$

So, although the interaction function J depends on the applied external fields, when $B_- \ll B_+$, we can make $J = J\left(B_+\right)$ and consider the vector $\mathbf{K}$ in (10) as composed of two independent functions $J\left(t\right)$ and $B_-\left(t\right)$. Besides, the interaction function can be controlled by electric fields [9, 11], whose interference in the spin states via the spin-orbit coupling, in many practical applications, can be neglected.

4. CONSTRUCTING THE XOR GATE

In this section we describe how the parameters of the parallel external fields can be chosen, so that the fields act as a XOR gate. As described in condition (1) in Sec. 1, the variations of the fields cannot be too fast so as to prevent the excitation of higher energy-levels. This problem can be avoided by using an *adiabatic variation* of the interaction, which can be obtained by a time-dependence in the form of $\operatorname{sech}\left(\omega t\right)$ [4]. A lot of solutions of this sech form can be found in [5]. Let us analyze, for example, a variation of the form

$$J\left(t\right) = \frac{a}{\cosh\omega t}, \quad B_- = c, \quad (13)$$

where a, c are constants and $\omega \ll \Delta E/\hbar$ (see condition (1) in Sec. 1). This interaction function will be turned off when $t \gg 1/\omega$. In this time limit the evolution operator (9), for the field (13), will behave as the operator (6) when the following conditions are met [8]:

$$\int_0^t B_+\left(\tau\right)\, d\tau = \frac{\pi}{2}\mathrm{mod}\left(2\pi\right), \ F\left(1+\lambda, 1-\lambda, \gamma+1; \frac{1}{2}\right) = 0, \quad (14)$$

where $F\left(\alpha, \beta, \gamma, z\right)$ is the Gauss hypergeometric function and the sum of fields $\left(B_+\right)$ is, besides the above condition, completely arbitrary.

For different fields at each dot, $B_- = c \neq 0$, the above conditions give the following restriction for the amplitude of the interaction function:

$$a = \frac{\omega\pi\,(1+4m)}{4\arctan\left[\exp\left(\omega T\right)\right] - \pi}, \quad T = \frac{n\pi}{c} \gg \frac{1}{\omega}, \quad n, m \in \mathbb{N}^*. \tag{15}$$

When the two dots are subject to the same field ($B_- = c = 0$), the second condition in (14) can be fixed using the relation $F\,(1+\lambda, 1-\lambda; 3/2; 1/2) = \lambda^{-1}\sin\left(\lambda\pi/2\right)$ [12], which gives

$$|a| = 2m\omega, \quad m \in \mathbb{N}^*. \tag{16}$$

The above relations fix the duration and the intensity of the fields for the adiabatic parallel pulse. The same analysis presented here can also be carried out for all the families of external fields presented in [5] and for different universal quantum gate.

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