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Rabi oscillations, coherent properties and model qubits in two-level donor systems under terahertz radiation

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Quantum confinement, magnetic-field effects, and laser coupling with the two low-lying states of electrons bound to donor impurities in semiconductors may be used to coherently manipulate the two-level donor system in order to establish the appropriate operational conditions of basic quantum bits (qubits) for solid-state based quantum computers. Here we present a detailed theoretical calculation of the damped Rabi oscillations and time evolution of the 1s and $2p_+$ donor states in bulk GaAs under an external magnetic field and in the presence of terahertz laser radiation, and their influence on the measured photocurrent. We also detail the possible experimental conditions under which decoherence is weak and qubit operations are efficiently controlled.

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Some two decades ago, it was suggested that quantum-mechanical computers (QC) might provide much more computing power than machines based on classical physics[1]. More recently, the discovery of fast quantum algorithms for tasks such as prime factorization and searching disordered databases[2] as well as quantum error correction codes[3] have arisen considerable interest in the search for suitable physical systems on which reliable quantum hardware could be realized. A precisely defined two-fold Hilbert space may be regarded as the base of a QC, under the conditions that decoherence is weak and single-qubit and two-qubit unitary operations are controlled.

Many implementations have been suggested for quantum computation involving manipulation of nuclear spin states in bulk solution using nuclear magnetic resonance techniques (NMR)[4], trapped ions[5], photons in microcavity[6], and specifically selected donor[7] or exciton[8–10] states in semiconductor systems as qubits to be manipulated by laser radiation. Solid-state proposals open up the possibility of fabricating large integrated networks that would be required for realistic applications of quantum computers. Two interesting suggestions for such semiconductor QCs are based on qubits using the spin of a phosporus donor nucleus in bulk silicon[11] and the spins of electrons trapped in a GaAs quantum dot (QD)[12,13]. Of course, a silicon-based computer is extremely attractive from many aspects but unfortunately difficulties concerning its practical realization have been pointed out recently[14]. The main problem is related to the strong oscillations in the exchange splitting- basic ingredient for the two-qubit operation in silicon-based QC, originated from degeneracy of the conduction band minimum in Si. This situation does not occur in GaAs where coupled-QD structures have been previously theoretically investigated[12,13,15] considering two coupled GaAs QDs. This corresponds essentially to "a 2D - hydrogen-like molecule", in the presence of an external magnetic field. An extensive study by Hu and Das Sarma[13] and de Sousa *et al*[15] suggested that the two-QD system would provide the necessary two-qubit entanglement required for QCs. In this case, the QDs provide the tag for each qubit which are represented by the spin of the QD-trapped electron, and single-qubit operations are performed on the tag-spin by a local external magnetic field or equivalently by an efficient manipulation of the local spin states[16]. The two-qubit operation, which rotates one of the tag-spin qubit in a precise angle if, and only if, the other control-qubit is oriented in a well defined unchanged direction, is realized via exchange interaction between the electrons in each QD. This means that in order to have a precise control of two-qubit operations it is necessary to fine-tune the exchange coupling through gates which are physically realized by external fields. One should note that a QC based on this architeture would be effective only if the spin decoherence time is much longer than the time involved in the single- and two-qubit operations, which could pose a problem, as these operations would be controlled by switching electric and/or magnetic fields and this cannot be performed very fast. It is possible to overcome this limitation if, instead of slow external gate potential and/or magnetic fields, one uses a laser-probe pulse to control the qubit operations. This can be achieved via coherent manipulation of two-level systems through Rabi oscillations in donor[7] or exciton[8–10] states, by applying electromagnetic fields. Cole *et al*[7] and Zrenner *et al*[10] have demonstrated that the coherent optical excitations in a QD and bulk GaAs two-level systems, respectively, can be converted into deterministic photocurrents. Here, the impurities (dots) provide the tag for each qubit which are represented by the two-level system. Moreover, it has been shown[17] that donor states in QDs, under magnetic and pump-laser[18] fields, may be properly manipulated in order to produce the required robust donor states for terahertz coherent manipulation of qubits. In the present work, we present a detailed theoretical calculation of the time evolution of the 1s and $2p_+$ donor states in bulk GaAs and their influence on the photocurrent[7], and thoroughly detail the conditions under which decoherence is weak.

A set of optical Bloch equations[18] is used to describe the time evolution of the elements of the density matrix within a two-level model for the impurity system, i.e.,

$$\begin{aligned}
\frac{d\rho_{11}}{dt} &= -i\Omega_R \cos(\omega_L t)(\rho_{21}-\rho_{12}) + \gamma_1\rho_{22} \\
\frac{d\rho_{22}}{dt} &= +i\Omega_R \cos(\omega_L t)(\rho_{21}-\rho_{12}) - (\gamma_1+\gamma_3)\rho_{22} \qquad (1) \\
\frac{d\rho_{12}}{dt} &= +i\omega_{21}\rho_{12} + i\Omega_R \cos(\omega_L t)(\rho_{11}-\rho_{22}) - \gamma_2\rho_{12} \\
\frac{d\rho_{21}}{dt} &= -i\omega_{21}\rho_{21} - i\Omega_R \cos(\omega_L t)(\rho_{11}-\rho_{22}) - \gamma_2\rho_{21}
\end{aligned}$$

where ω_L is the THz laser frequency, ω_{21} is the energy separation of the 1s and $2p_+$ impurity levels, $\Omega_R = E_{THz} d^x_{12}/\hbar$ is the Rabi frequency, E_{THz} is the amplitude of the terahertz electric field (in the x-direction), and d^x_{12} is the x-component of the 1s-$2p_+$ dipole matrix element[19]. The parameters γ_1, γ_2, and γ_3 are recombination rates as defined in Cole *et al*[7]. The 1s- and $2p_+$-like impurity states are calculated by using hydrogenic-like wave functions with exponentially-decaying variational parameters taken as λ_{1s} and λ_{2p_+}. The calculated energies, in effective units, are given by

$$\epsilon_{1s} = E_c + \frac{1}{\lambda_{1s}^2} - \frac{2}{\lambda_{1s}} + \frac{1}{2}\gamma^2\lambda_{1s}^2 \ , \qquad (2)$$

$$\epsilon_{2p_+} = E_c + \frac{1}{\lambda_{2p_+}^2} - \frac{1}{\lambda_{2p_+}} + \gamma + \frac{3}{2}\gamma^2\lambda_{2p_+}^2 \ , \qquad (3)$$

where $E_c = E_c^o + \gamma$, E_c being the magnetic-field dependent conduction-band edge, and $\gamma = e\hbar B/2m^*cR^*$ is the effective magnetic energy, with $R^* \approx 5.9\ meV$ the GaAs effective Rydberg. The parameters λ_{1s} and λ_{2p_+} are obtained variationally as a function of the applied magnetic field (in the z-direction). Fig. 1(a) shows the energies of both impurity states together with the magnetic-field dependence of the energy of the conduction-band edge. By using the value of $\nu = 2.52\ THz$ for the radiation frequency as in the experiment by Cole *et al*[7], we calculated the magnetic field value of 3.4 T for which the 1s-$2p_+$ transition is tuned with the radiation. This is in good agreement with the experimental value of 3.51 T obtained by Cole *et al*[7] at very low values of the terahertz electric field. The 1s and $2p_+$ hydrogenic-like wave functions, for the impurity under a magnetic field of 3.4 T, are used to theoretically evaluate the Rabi frequency as a function of the THz electric field, and results are shown as a full curve in Fig. 1(b). Also shown are the fit parameters by Cole *et al*[7] as full triangles. We note that Cole *et al*[7] have pointed out that the uncertainty of the absolute scale of E_{THz} is ± 50 % and the uncertainty in relatives values of E_{THz} is negligible. With this in mind, one observes that the open triangles, which correspond to a horizontal shift of the fit parameters by 1.1 x 10^4 Vm^{-1}, are in quite good agreement with our theoretical prediction for the Rabi frequency.

The equations of motion of the density matrix may be solved via the rotating-wave scheme[18], and solutions essentially oscillate with a frequency close to the Rabi frequency, with damping terms depending on the various recombination mechanisms. To discuss the photocurrent measurements in Fig. 4(a) of Cole *et al*[7], we choose γ_1=0, γ_2 = 1.5 x 10^{11} rad s^{-1}, γ_3 = 1.0 x 10^{11} rad s^{-1}, and Ω_R = 3.0 x 10^{11} rad s^{-1}. Our calculated results for the photocurrent [taken as proportional to $1-\rho_{11}(t)$] in Fig. 2(a) show that this choice of parameters fits quite well their experimental data for the photocurrent, in the range of measured detunings. Note that the theoretical photocurrent results in Fig. 2(a) indicate [cf. Fig. 1(b)] that the experimental data in Fig. 4(a) of Cole *et al*[7] should be assigned to a laser amplitude of $E_{THz} \approx$ 3.1 x 10^4 Vm^{-1}. In Fig. 2(b), we display the theoretical photocurrent for a laser detuning δ= -0.014 THz as compared with $\rho_{22}(t)$ (number of donors at the $2p_+$ state), and $\rho_{11}(t) + \rho_{22}(t)$ (total population in the 1s and $2p_+$ states). One notes that the populations of both the 1s and $2p_+$ states have a fast decrease with pulse duration. Therefore, it is clear that the measured photocurrent may have a dominant contribution from the charge ionized from the $2p_+$ state into the conduction band, making the existence of coherent Rabi oscillations more difficult to be observed, *i.e.*, the fact that the $2p_+$ state is immersed in the conduction band results in a strong decoherence process. It is important to mention here that it is possible to increase the confinement of the donor electrons by trapping the impurities in QDs or via the use of a pump-laser tuned below the semiconductor gap, in order to lower the energy of the $2p_+$ state and to bring it below the conduction-band continuum[17]. This situation corresponds to a choice of the γ_3 ionization rate equal to zero, as shown for the calculated photocurrent in Fig. 3(a). Alternatively, one may efficiently control the decoherence process through a diluted doping procedure in which the inhomogeneous broadening of the 1s-$2p_+$ transition energy is conveniently reduced. This occurs because the overlap between the impurity wave functions diminishes. Again, the confinement of the electronic states via a pump-laser field may be used to mimic this effect. Such behaviour may be modelled by assuming the total dephasing rate $\gamma_2 = 0$, as displayed in Fig. 3(b). One should note that a too low impurity concentration may result in a weak photosignal which is a rather undesirable experimental situation. In the theoretical photocurrent displayed in Fig. 3(c), it is quite clear the obvious fundamental role played by the strength of the electromagnetic field, through the Rabi oscillations, on the coherence process.

In conclusion, we have obtained the solutions of the optical Bloch equations within the rotating-wave approximation in order to discuss the proposal of Cole *et al*[7]. The donor 1s and $2p_+$ hydrogenic-like states, in the presence of a homogeneous magnetic field, are obtained through a variational procedure. Theoretical calculations have shown that the resonance condition - for which the 1s-$2p_+$ transition is tuned with the terahertz radiation - is achieved for a magnetic field in good agreement with the measured experimental value. Moreover, the theoretical results obtained for the THz electric field-dependence of the Rabi frequencies are found in excellent agreement with the experimentally fitted curve, provided that the uncertainty of the absolute experimental scale for the electric field is taken into account. The theoretical calculations concerning the time-dependent behaviour of the photocurrent, a fundamental observable for an efficient determination of qubit operations, show that it is dominated by the ionized charge in the conduction band, and that this effect relates to the $2p_+$ state being immersed in the conduction band. In that respect, we have detailed the possible experimental conditions for which decoherence effects are minimized so that qubit operations are efficiently controlled.

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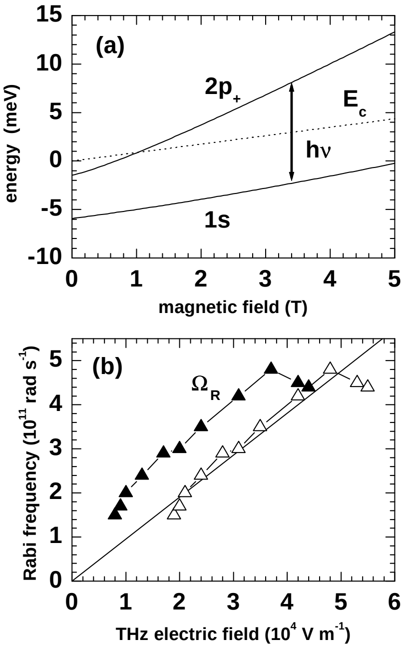

FIG. 1. (a) Theoretical magnetic - field dependence of the 1s and $2p_+$ donor states together with the field-dependence of the GaAs E_c conduction-band edge. At 3.4 T, one obtains a 1s-$2p_+$ transition tunable to an energy corresponding to 2.52 THz; (b) Rabi frequency as a function of the THz electric field (full curve), obtained via a variational calculation (see text). Full triangles are the fit parameters by Cole *et al*[7], with open triangles corresponding to a horizontal shift by 1.1 x 10^4 Vm^{-1}.

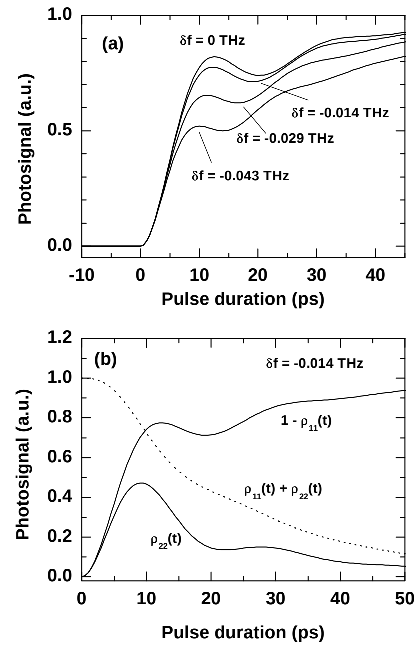

FIG. 2. (a) Theoretical $1-\rho_{11}(t)$ photocurrent (arbitrary units) as a function of pulse duration for various laser detunings δ=0 THz, -0.014 THz, -0.029 THz, and -0.043 THz; (b) Photocurrent for a laser detuning δ= -0.014 THz as compared with $\rho_{22}(t)$ (number of donors at the $2p_+$ state), and $\rho_{11}(t)+\rho_{22}(t)$. Results are calculated using γ_1=0, γ_2 = 1.5 x 10^{11} rad s^{-1}, γ_3 = 1.0 x 10^{11} rad s^{-1}, and Ω_R = 3.0 x 10^{11} rad s^{-1}.

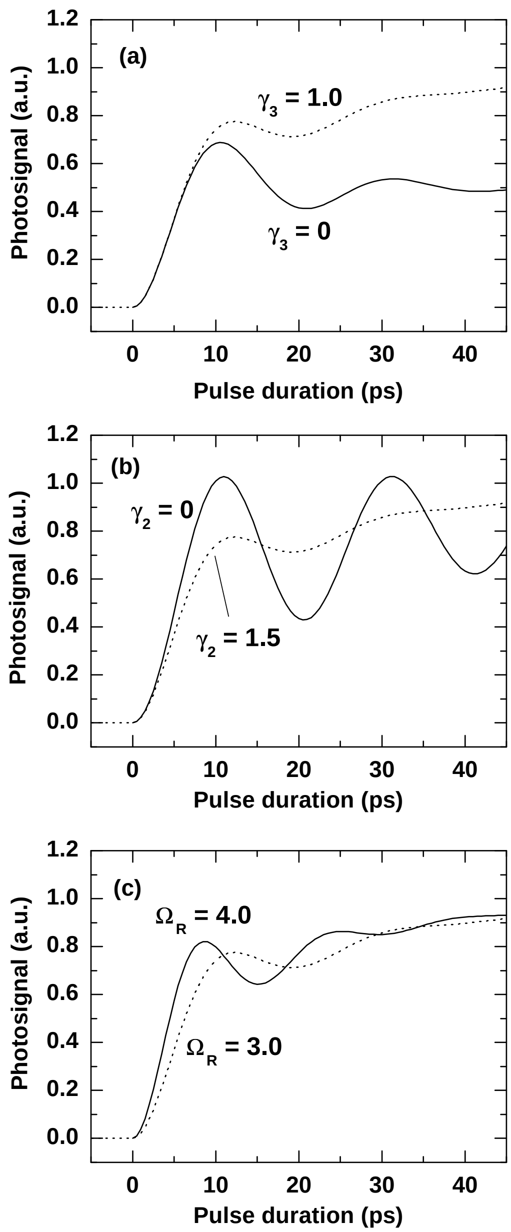

FIG. 3. Dependence of the photocurrent (arbitrary units) on the pulse duration for a fixed laser detuning $\delta =$ -0.014 THz and (a) $\gamma_3 = 0$, and $\gamma_3 = 1.0$ (with $\gamma_2 = 1.5$ and $\Omega_R = 3.0$), (b) $\gamma_2 = 0$, and $\gamma_2 = 1.5$ (with $\gamma_3 = 1.0$ and $\Omega_R = 3.0$); and (c) $\Omega_R = 3.0$, and $\Omega_R = 4.0$ (with $\gamma_2 = 1.5$ and $\gamma_3 = 1.0$). Rabi frequencies and rate parameters are given in units of 10^{11} rad s^{-1}.