Phonon-induced decoherence of the two-level quantum subsystem
due to relaxation and dephasing processes

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ABSTRACT

Phonon-related decoherence effects in a quantum double-well two-level subsystem coupled to
a solid are studied theoretically by the example of deformation phonons. Expressions for the
reduced density matrix at $T = 0$ are derived beyond the Markovian approximation by means of
explicit solution of the non-stationary Schrödinger equation for the interacting electron-phonon
system at the initial stage of its evolution. It is shown that as long as the difference between
the energies of the electron in the left and the right well greatly exceeds the energy of the
electron tunneling between the minima of the double-well potential, decoherence is primarily
due to dephasing processes. This case corresponds to a strongly asymmetric potential and
spatially separated eigenfunctions localized in the vicinity of one or another potential minimum.
In the opposite case of the symmetric potential, the decoherence stems from the relaxation
processes, which may be either ”resonant” (at relatively long times) or "nonresonant" (at short
times), giving rise to qualitatively different temporal evolution of the electron state. The results
obtained are discussed in the context of quantum information processing based on the quantum
bits encoded in electron charge degrees of freedom.

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I. INTRODUCTION

Recent advances in fabrication of the quantum dot structures [1], manipulation with the single atoms on a solid surface [2], and atomically precise placement of single dopants in semiconductors [3-4] make possible the construction of various solid-state architectures with predetermined characteristics. The state-of-the-art experimental techniques allow for a control of the quantum states of charge carriers in nanostructures [5-9]. A number of interesting phenomena have been observed and predicted, including Rabi oscillations [10], the entanglement between the states of interacting quantum dots [11], complete localization of the wave packet in one of the wells of a symmetric double-well potential perturbed by a monochromatic driving force [12], the auxiliary-level-assisted electron transfer between the quantum dots [13-14], localization of two interacting electrons in a driven quantum dot molecule [15], coherent control of tunneling in a quantum dot molecule [16], etc.

The coupling of carriers to the surrounding crystal lattice results in entanglement between the carrier and lattice degrees of freedom and in the loss of coherence [17]. In experiment, decoherence of quantum states can lead to, e. g., decay of coherent optical polarization [10], damping of Rabi oscillations [18], errors in operations on the quantum bits (qubits) [19], etc. In theory, decoherence manifests itself in the temporal decay of the reduced density matrix elements. There exist different approaches to the description of decoherence effects in solids, see, e. g., Refs. [17, 20-24].

In this paper, we study the phonon-related decoherence of a two-level quantum subsystem within a solid by means of solution of the non-stationary Schrödinger equation for the interacting carrier-lattice system. We obtain an explicit expression for the state vector and find the reduced density matrix taking a trace over the phonon variables. Decoherence is shown to be primarily due to either dephasing or relaxation processes, depending on the specific structure of the
energy basis and eigenfunctions of the two-level subsystem.

The paper is organized as follows. In Section II, we describe a model for the two-level subsystem coupled to a solid. In Section III, we present an approximate solution of the time-dependent Schrödinger equation for the interacting electron-reservoir system at zero temperature. An expression for the reduced density matrix of the two-level subsystem is derived in Section IV, and several limiting cases are considered by the example of the double-dot structure. The results are discussed in Section V, and Section VI concludes the paper.

II. MODEL FOR THE TWO-LEVEL SUBSYSTEM COUPLED TO A SOLID

We consider an electron in a double-well potential formed in a solid. Such a subsystem corresponds to, e. g., the gate-engineered double-dot structure [25], two nearby donors beneath the semiconductor surface [26], etc. We suppose that the two lowest states of the electron, \(|1\rangle\) and \(|2\rangle\), are well separated in energy from the excited states \(|k\rangle\) with \(k \geq 3\). Then the electron Hamiltonian can be written as

\[
\hat{H}_0 = E_1 |1\rangle \langle 1| + E_2 |2\rangle \langle 2| ,
\]

where \(E_1\) and \(E_2\) are the eigenenergies of the stationary Schrödinger equation

\[
\hat{H}_0 |k\rangle = E_k |k\rangle .
\]

For the subsequent consideration, it is instructive to write the Hamiltonian \(\hat{H}_0\) in the basis \(\{|L\rangle, |R\rangle\}\) formed by the ground states of the electron in the left and the right well in the case that the wells are isolated from each other. We assume the wave functions \(\langle r|L\rangle\) and \(\langle r|R\rangle\) to be strongly localized in the vicinity of the corresponding potential minima. Then, neglecting
the overlap $\langle L|R\rangle$, we have

$$\hat{H}_0 = E_L |L\rangle \langle L| + E_R |R\rangle \langle R| - \frac{\Delta}{2} \left( |L\rangle \langle R| + |R\rangle \langle L| \right), \tag{3}$$

where $E_L$ and $E_R$ are the energies of the states $|L\rangle$ and $|R\rangle$ localized in the vicinity of, respectively, the left and the right potential minimum, and $\Delta/2$ is the energy of the electron tunneling between the two minima.

The states $|1\rangle$ and $|2\rangle$ are related to the states $|L\rangle$ and $|R\rangle$ by the following expressions

$$|1\rangle = C_- |L\rangle + C_+ |R\rangle, \quad |2\rangle = C_+ |L\rangle - C_- |R\rangle, \tag{4}$$

where

$$C_\pm = \frac{1}{\sqrt{2}} \left[ 1 \pm \frac{E_L - E_R}{\sqrt{(E_L - E_R)^2 + \Delta^2}} \right]. \tag{5}$$

The relation between $E_{1,2}$ and $E_{L,R}$ is

$$E_{1,2} = E_L + E_R \mp \sqrt{(E_L - E_R)^2 + \Delta^2}. \tag{6}$$

In what follows, we shall consider the limiting cases of (i) the strongly asymmetric potential, i. e., $E_R - E_L \gg \Delta$, so that we assume $\Delta = 0$, and (ii) the symmetric potential, i. e., $E_L = E_R$ and $\Delta \neq 0$. From Eqs. (4)-(6) one has

$$|1\rangle = |L\rangle, \quad |2\rangle = |R\rangle, \quad E_{1,2} = E_{L,R} \tag{7}$$

in the case (i) and

$$|1\rangle = \frac{|L\rangle + |R\rangle}{\sqrt{2}}, \quad |2\rangle = \frac{|L\rangle - |R\rangle}{\sqrt{2}}, \quad E_{1,2} = \frac{E_L + E_R \mp \Delta}{2} = E_L \mp \frac{\Delta}{2} \tag{8}$$

in the case (ii).

The phonon term in the Hamiltonian is (hereafter the Planck constant $\hbar = 1$ if not stated explicitly)

$$\hat{H}_{ph} = \sum_\beta \omega_\beta \left( \hat{b}_\beta^+ \hat{b}_\beta + \frac{1}{2} \right), \tag{9}$$
where $\omega_\beta$ is the frequency of the phonon mode $\beta = (\mathbf{q}, \lambda)$ with the wave vector $\mathbf{q}$ and polarization $\lambda$, and $\hat{b}_\beta^+ (\hat{b}_\beta)$ is the creation (annihilation) operator of the phonon of the mode $\beta$. The eigenstates $|\{n_\beta\}\rangle$ of the stationary Schrödinger equation

$$\hat{H}_{ph}|\{n_\beta\}\rangle = E(\{n_\beta\})|\{n_\beta\}\rangle \quad (10)$$

are defined by the set $\{n_\beta\}$ of the phonon numbers $n_\beta$ for every mode $\beta$, the eigenenergies being equal to

$$E(\{n_\beta\}) = \sum_\beta \omega_\beta \left( n_\beta + \frac{1}{2} \right). \quad (11)$$

The electron-phonon interaction term is

$$\hat{H}_{int} = \sum_\beta \left[ \lambda_\beta \hat{\rho}(\mathbf{q}) \hat{b}_\beta^+ + \lambda_\beta^* \hat{\rho}^+(\mathbf{q}) \hat{b}_\beta \right], \quad (12)$$

where $\hat{\rho}(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} \hat{\rho}(\mathbf{r})$ is the Fourier transform of the electron density operator $\hat{\rho}(\mathbf{r}) = \sum_{mn} \Psi_m^*(\mathbf{r}) \Psi_n(\mathbf{r}) |m\rangle \langle n|$, and $\lambda_\beta$ is the microscopic electron-phonon interaction matrix element, which can be expressed in terms of the deformation potential $\Xi$ and the density of the crystal $\rho$ as (here we restrict ourselves to deformation phonons)

$$\lambda_\beta = q \Xi \left( \frac{\hbar}{2\rho \omega_\beta V} \right)^{1/2}, \quad (13)$$

with $V$ being the normalizing volume. The Hamiltonian (12) can be written in the spin-boson form as [27]

$$\hat{H}_{int} = \hat{\sigma}_z \sum_\beta \left[ g_\beta \hat{b}_\beta^+ + g_\beta^* \hat{b}_\beta \right], \quad (14)$$

where $\hat{\sigma}_z = |L\rangle \langle L| - |R\rangle \langle R|$ is the Pauli spin operator in the basis $\{|L\rangle, |R\rangle\}$,

$$g_\beta = \frac{\lambda_\beta}{2} \left[ A_L(\mathbf{q}) - A_R(\mathbf{q}) \right], \quad (15)$$

and $A_{L,R}(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} |\langle \mathbf{r} | L, R \rangle|^2$. 

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To be specific, in what follows we consider the double-dot system with the Gaussian-shaped electron wave functions $\langle r | L, R \rangle \sim \exp(-|r - r_{L,R}|^2/2l^2)$, where $r_{L,R}$ are the coordinates of the dot centers, and $l$ is the effective dot size. Then from Eq. (15) one has \[ g_\beta = i\lambda_\beta \exp \left(-\frac{q^2d^2}{4}\right) \sin \left(\frac{qd}{2}\right), \] (16)

where $d = r_R - r_L$ (i.e., $d$ is the interdot distance), and we choose the origin of the coordinates in between the dots. Note that the condition of vanishingly small overlap $\langle L | R \rangle$ implies that $l << d$. From Eqs. (13) and (16) we find the spectral density $J(\omega)$ that fully describes the effect of the phonon bath on the two-level electron subsystem \[ J(\omega) = \sum_\beta |g_\beta|^2 \delta(\omega_\beta - \omega) = \frac{\Xi^2\hbar}{8\pi^2\rho s^5} \omega_\beta^3 \left[1 - \frac{\omega_d}{\omega} \sin \left(\frac{\omega}{\omega_d}\right)\right] \exp \left(-\frac{\omega^2}{2\omega_l^2}\right), \] (17)

where we assumed the linear dispersion law $\omega_q = sq$ with $s$ being the sound velocity and used the notations $\omega_d = s/d$ and $\omega_l = s/l$ from Ref. \[28\] (note that $\omega_l >> \omega_d$).

### III. STATE VECTOR OF THE INTERACTING SYSTEM

The state vector $|\Psi(t)\rangle$ of the interacting electron-phonon system satisfies the non-stationary Schrödinger equation \[ i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \hat{H} |\Psi(t)\rangle, \] (18)

where \[ \hat{H} = \hat{H}_0 + \hat{H}_{ph} + \hat{H}_{int} \] (19)

is the full Hamiltonian. The state vector can be represented as a linear combination of products of the electron and phonon states, \[ |\Psi(t)\rangle = \sum_{k=1,2} \sum_{\{n_\beta\}} C_{k,\{n_\beta\}}(t) e^{-iE_k t - iE(\{n_\beta\}) t} |k\rangle |\{n_\beta\}\rangle. \] (20)
Note that in the absence of the electron-phonon interaction, the coefficients $C_{k,\{n_\beta\}}$ do not depend on time. We consider the case of zero temperature, so that initially there are no phonons in the solid ($n_\beta = 0$ for any mode $\beta$), while the electron is in the superpositional state $\alpha_L |L\rangle + \alpha_R |R\rangle$, where $|\alpha_L|^2 + |\alpha_R|^2 = 1$, and hence the state vector at $t = 0$ is

$$|\Psi(0)\rangle = \left(\alpha_L |L\rangle + \alpha_R |R\rangle\right)|0_{ph}\rangle,$$  \hspace{1cm} (21)

where $|0_{ph}\rangle$ is the state without phonons, or, equivalently,

$$C_{L,0_{ph}}(0) = \alpha_L, \quad C_{R,0_{ph}}(0) = \alpha_R, \quad C_{k,\{n_\beta\neq0\}}(0) = 0.$$  \hspace{1cm} (22)

[Relation between the coefficients $C_{1,\{n_\beta\}}(t)$, $C_{2,\{n_\beta\}}(t)$ and $C_{L,\{n_\beta\}}(t)$, $C_{R,\{n_\beta\}}(t)$ depends on the relation between the states $|1\rangle$, $|2\rangle$ and $|L\rangle$, $|R\rangle$ which is different in the cases (i) and (ii), see Eqs. (7) and (8)].

Substituting Eq. (20) into Eq. (18), we have a system of coupled differential equations for coefficients $C_{k,\{n_\beta\}}(t)$,

$$i\frac{dC_{k,\{n_\beta\}}(t)}{dt} e^{-iE_k t - iE(|\{n_\beta\}|) t} = \sum_{l=1,2} \sum_{\{m_\beta\}} C_{l,\{m_\beta\}}(t) \langle k | \hat{\sigma}_z | l \rangle \langle \{n_\beta\} | \hat{H}_{int} | l \rangle \langle \{m_\beta\} \rangle e^{-iE_l t - iE(|\{m_\beta\}|) t}. \hspace{1cm} (23)$$

From Eq. (14) we find

$$\langle \{n_\beta\} | \langle k | \hat{H}_{int} | l \rangle \langle \{m_\beta\} \rangle \rangle = \langle k | \hat{\sigma}_z | l \rangle \sum_{\beta'} g_{\beta'} \sqrt{m_{\beta'}} + 1 \delta_{\{m_\beta\},\{n_\beta\}-1,\beta'} + g_{\beta'}^* \sqrt{m_{\beta'}} \delta_{\{m_\beta\},\{n_\beta\}+1,\beta'}, \hspace{1cm} (24)$$

where the designation $\{n_\beta\} \pm 1,\beta'$ means the set of the phonon numbers with one phonon of the mode $\beta'$ more/less than in the set $\{n_\beta\}$. With this expression, Eq. (23) becomes

$$i\frac{dC_{k,\{n_\beta\}}(t)}{dt} = \sum_{l=1,2} \sum_{\beta'} \langle k | \hat{\sigma}_z | l \rangle \sum_{\beta'} \left[C_{l,\{n_\beta\}-1,\beta'}(t) g_{\beta'} \sqrt{m_{\beta'}} e^{i\omega_{\beta'} t} + \right.$$  

$$+ C_{l,\{n_\beta\}+1,\beta'}(t) g_{\beta'}^* \sqrt{m_{\beta'}} + 1 e^{-i\omega_{\beta'} t} \right]. \hspace{1cm} (25)$$
where we took into account that \( E(\{n_\beta\} \pm 1,_{\beta'}) = E(\{n_\beta\}) \pm \omega_{\beta'} \). From Eq. (25) we have

\[
\frac{dC_{k,0ph}(t)}{dt} = \sum_{l=1,2} \langle k|\hat{\sigma}_z|l\rangle e^{-i(E_l - E_k)t} \sum_{\beta} C_{l,1,\beta}(t) g_\beta e^{-i\omega_{\beta}t}
\]

and

\[
\frac{dC_{k,1,\beta}(t)}{dt} = \sum_{l=1,2} \langle k|\hat{\sigma}_z|l\rangle e^{-i(E_l - E_k)t} \left[ C_{l,0ph}(t) g_\beta e^{i\omega_{\beta}t} + \sum_{\beta'} C_{l,1,\beta'}(t) g_{\beta'} e^{-i\omega_{\beta}t} \right].
\]

We wish to consider either the initial stage of the system evolution or the case of "weak decoherence", so that the state vector \(|\Psi(t)\rangle\) does not differ much from \(|\Psi(0)\rangle\). This implies that all coefficients \(C_{k,(n_\beta)}(t)\) in \(|\Psi(t)\rangle\) except \(C_{k,0ph}(t)\) are small and decrease with the number of phonons \(\sum_\beta n_\beta\) in the state \(\{n_\beta\}\), and hence, in the first approximation

\[
|\Psi(t)\rangle \approx \sum_{k=1,2} C_{k,0ph}(t) e^{-iE_k t} - i E_{0ph} t |k\rangle|0ph\rangle + \sum_{k=1} C_{k,1,\beta}(t) e^{-iE_k t - i\omega_{\beta} t - i E_{0ph} t} |k\rangle|1_\beta\rangle,
\]

where \(E_{0ph} = \sum_\beta \omega_{\beta}/2\) is the zero-point phonon energy. Neglecting the second (two-phonon) term in the right-hand side of Eq. (27), taking \(C_{l,0ph}(t) \approx C_{l,0ph}(0)\), and integrating Eq. (27), we have

\[
C_{k,1,\beta}(t) \approx g_\beta \sum_{l=1,2} C_{l,0ph}(0) \langle k|\hat{\sigma}_z|l\rangle \frac{e^{-i(E_l - E_k - \omega_{\beta}) t} - 1}{E_l - E_k - \omega_{\beta}}.
\]

Substituting this expression into Eq. (26) and evaluating the integral, we have

\[
C_{k,0ph}(t) \approx C_{k,0ph}(0) + \sum_{l=1,2} \sum_{m=1,2} C_{m,0ph}(0) \langle k|\hat{\sigma}_z|l\rangle \langle l|\hat{\sigma}_z|m\rangle \sum_\beta \left| g_\beta \right|^2 \frac{1}{E_m - E_l - \omega_{\beta}} \left( \frac{e^{-i(E_m - E_k) t} - 1}{E_m - E_k} - \frac{e^{-i(E_l - E_k + \omega_{\beta}) t} - 1}{E_l - E_k + \omega_{\beta}} \right).
\]

Now let us analyze the expressions for \(C_{k,0ph}(t)\) and \(C_{k,1,\beta}(t)\) in the limiting cases (i) and (ii) mentioned in Sec. II.

(i) Strongly asymmetric double-well potential \((E_L \neq E_R, \Delta = 0)\)
In this case, we have from Eqs. (7)

\[ \langle 1 | \hat{\sigma}_z | 1 \rangle = 1, \quad \langle 2 | \hat{\sigma}_z | 2 \rangle = -1, \quad \langle 1 | \hat{\sigma}_z | 2 \rangle = \langle 2 | \hat{\sigma}_z | 1 \rangle = 0, \]

so that Eqs. (29) and (30) become

\[ C_{k,1\beta}(t) \approx (-1)^k C_{k,0\beta}(0) g_{\beta} \frac{e^{i\omega_{\beta}t} - 1}{\omega_{\beta}}, \]

\[ C_{k,0\beta}(t) \approx C_{k,0\beta}(0) \left[ 1 + \sum_{\beta} \left| g_{\beta} \right|^2 \frac{\omega_{\beta}^2}{\omega_{\beta}} \left( i\omega_{\beta}t + e^{-i\omega_{\beta}t} - 1 \right) \right]. \]

It follows from Eq. (33) that the quantitative conditions for our approximation \( C_{k,0\beta}(t) \approx C_{k,0\beta}(0) \) are:

\[ \Lambda \equiv \sum_{\beta} \frac{|g_{\beta}|^2}{\hbar^2 \omega_{\beta}^2} = \int_0^\infty d\omega \frac{J(\omega)}{\hbar^2 \omega} \ll 1 \]

and

\[ t \ll t_0 \equiv \left[ \sum_{\beta} \frac{|g_{\beta}|^2}{\hbar^2 \omega_{\beta}^2} \right]^{-1} = \left[ \int_0^\infty d\omega \frac{J(\omega)}{\hbar^2 \omega} \right]^{-1}. \]

For the spectral function given by Eq. (17) one has (the second term in square brackets of Eq. (17) can be neglected since \( \omega_l >> \omega_d \)):

\[ \Lambda \approx \frac{\Xi^2}{8\pi^2 \rho s^3 l^2 \hbar} \sim \frac{J(\omega_l)}{\hbar^2 \omega_l}, \]

\[ t_0 \approx 8\pi \sqrt{2\pi \frac{\rho s^3 l^3 \hbar}{\Xi^2}} \sim \frac{1}{\Lambda \omega_l}. \]

For the parameters of GaAs (\( \Xi \approx 7 \text{ eV}, s = 5.1 \cdot 10^5 \text{ cm/s}, \rho = 5.3 \text{ g/cm}^3 \)) we have \( \Lambda \approx 3 \cdot 10^{-4} \) and \( t_0 \approx 10^{-8} \text{ s} \) at \( l = 25 \text{ nm} \). Note that \( \Lambda \) decreases with \( l \), while \( t_0 \) increases, so that our approach works better (and in a broader time interval) for relatively large quantum dots. For example, \( \Lambda \approx 2 \cdot 10^{-5} \) and \( t_0 \approx 7 \cdot 10^{-7} \text{ s} \) at \( l = 100 \text{ nm} \) (approximate dot size in Ref. [6]).

(ii) **Symmetric double-well potential** (\( E_L = E_R, \Delta \neq 0 \))
Now it follows from Eqs. (38) that

\[ \langle 1 | \hat{\sigma}_z | 1 \rangle = \langle 2 | \hat{\sigma}_z | 2 \rangle = 0 , \quad \langle 1 | \hat{\sigma}_z | 2 \rangle = \langle 2 | \hat{\sigma}_z | 1 \rangle = 1 , \tag{38} \]

and from Eqs. (29) and (30) we have

\[ C_{1,1}\beta(t) \approx -C_{2,0\text{ph}}(0) g_\beta \frac{e^{i(\omega_\beta - \Delta)t} - 1}{\omega_\beta - \Delta} , \tag{39} \]

\[ C_{2,1}\beta(t) \approx -C_{1,0\text{ph}}(0) g_\beta \frac{e^{i(\omega_\beta + \Delta)t} - 1}{\omega_\beta + \Delta} , \tag{40} \]

\[ C_{1,0\text{ph}}(t) \approx C_{1,0\text{ph}}(0) \left[ 1 + \sum_\beta \frac{|g_\beta|^2}{(\omega_\beta + \Delta)^2} \left( i(\omega_\beta + \Delta)t + e^{-i(\omega_\beta + \Delta)t} - 1 \right) \right] , \tag{41} \]

\[ C_{2,0\text{ph}}(t) \approx C_{2,0\text{ph}}(0) \left[ 1 + \sum_\beta \frac{|g_\beta|^2}{(\omega_\beta - \Delta)^2} \left( i(\omega_\beta - \Delta)t + e^{-i(\omega_\beta - \Delta)t} - 1 \right) \right] . \tag{42} \]

At \( \Delta \ll \omega_\ell \) (i.e., for well separated quantum dots), the conditions that coefficients \( C_{k,0\text{ph}}(t) \) do not differ much from their initial values \( C_{k,0\text{ph}}(0) \) are the same as in the case \((i)\), see Eqs. (34) and (35).

\section*{IV. DENSITY MATRIX}

Having found the state vector \( |\Psi(t)\rangle \) of the interacting electron-phonon system, we can calculate the reduced density matrix of the two-level electron subsystem by tracing out the phonon variables. From Eq. (20) we have

\[ \hat{\rho}(t) = Tr_{\{n_\beta\}} |\Psi(t)\rangle \langle \Psi(t)| = \sum_{\{n_\beta\}} \sum_{k=1,2} \sum_{l=1,2} e^{-i(E_k - E_l)t} C_{k,\{n_\beta\}}(t) C_{l,\{n_\beta\}}^* (t) \langle k | \langle l | . \tag{43} \]

According to approximations made in Sec. III, see Eq. (28), we retain in the sum over \( \{n_\beta\} \) the zero- and one-phonon terms only, so that the matrix elements of \( \hat{\rho}(t) \) in the energy basis read

\[ \rho_{kl}(t) \approx e^{-i(E_k - E_l)t} \left[ C_{k,0\text{ph}}(t) C_{l,0\text{ph}}^*(t) + \sum_\beta C_{k,1\beta}(t) C_{l,1\beta}^*(t) \right] . \tag{44} \]
Following the consideration in Sec. III, below we calculate \( \rho_{kl}(t) \) in two limiting cases (\( i \)) and (\( ii \)).

\( (i) \) Strongly asymmetric double-well potential (\( E_L \neq E_R, \Delta = 0 \))

Substituting expressions (32) and (33) into Eq. (44), and neglecting the terms containing \(|g_\beta|^4\) (i.e., the terms of the order of \( \Lambda^2, (t/t_0)^2, \) and \( \Lambda(t/t_0) \)), we have

\[
\hat{\rho}(t) \approx \left( \begin{array}{cc} \rho_{11}(0) & \rho_{12}(0) [1 - B^2(t)] e^{i(E_2 - E_1)t} \\ \rho_{21}(0) [1 - B^2(t)] e^{-i(E_2 - E_1)t} & \rho_{22}(0) \end{array} \right), \quad (45)
\]

where \( \rho_{kl}(0) = C_{k,0,ph}(0)C^*_{l,0,ph}(0) \) and

\[
B^2(t) = 8 \sum_{\beta} \frac{|g_\beta|^2}{\omega_\beta^2} \sin^2 \left( \frac{\omega_\beta t}{2} \right) = 8 \int_0^\infty \! d\omega \frac{J(\omega)}{\omega^2} \sin^2 \left( \frac{\omega t}{2} \right). \quad (46)
\]

(Here we use the notations of Refs. [19, 21, 29].) The value of \( B^2(t) \) equals to zero at \( t = 0 \) and increases with \( t \) as \( B^2(t) \approx 4\Lambda(\omega_l)^2 \) at \( t << \omega_l^{-1} \) (the value of \( \omega_l^{-1} \) is about \( 2 \cdot 10^{-11} \) s at \( l = 100 \) nm) up to \( B^2(t) \approx 4\Lambda \) at \( t >> \omega_l^{-1} \) (this is consistent with the range of validity of our approximation, \( t << t_0 \), since \( t_0 \sim 1/\Lambda \omega_l >> \omega_l^{-1} \)).

Since in this case \( |1\rangle = |L\rangle \) and \( |2\rangle = |R\rangle \), we arrive at the conclusion that electron-phonon interaction has no effect on the diagonal matrix elements \( \rho_{LL} \) and \( \rho_{RR} \), while the absolute values of the non-diagonal matrix elements \( \rho_{LR} \) and \( \rho_{RL} \) decrease with time. So, there is no relaxation in the system (i.e., occupations of both dots do not change during the system evolution), and decoherence emerges as pure dephasing, in accordance with the results of Ref.[19] and ”semiclassical” approach to electron-phonon interaction in the two-level systems [30]. The reason for this is that in the case of strongly asymmetric double-well potential, the electron Hamiltonian \( \hat{H}_0 \) commutes with the interaction Hamiltonian \( \hat{H}_{int} \), see Eqs. (11) and (14). Contrary to the results obtained in Refs. [21, 29], our expression (45) for \( \hat{\rho}(t) \) contains the factor \( 1 - B^2(t) \) instead of \( e^{-B^2(t)} \). This is a consequence of our approximations. Indeed, \( B^2(t) \leq 4\Lambda << 1, \) so
that $e^{-B^2(t)} \approx 1 - B^2(t)$. For times $t >> \omega_l^{-1}$ we have $B^2(t) \approx 4\Lambda$, i.e., the dephasing process does not depend on time.

(ii) Symmetric double-well potential ($E_L = E_R, \Delta \neq 0$)

Substituting expressions (39), (40), (41), (42) into Eq. (44), and neglecting, as above, the terms of the order of $|g_\beta|^4$, we obtain the density matrix elements in the energy basis:

\[
\rho_{11}(t) = 1 - \rho_{22}(t) \approx \rho_{11}(0) \left(1 - 4F_+(t)\right) + 4\rho_{22}(0)F_-(t),
\]

\[
\rho_{12}(t) = \rho_{21}(t) \approx \rho_{12}(0)e^{i\Delta t} \left[1 + \sum_\beta \frac{|g_\beta|^2}{\left(\omega_\beta + \Delta\right)^2} \left(i(\omega_\beta + \Delta)t + e^{-i(\omega_\beta + \Delta)t} - 1\right) + \sum_\beta \frac{|g_\beta|^2}{\left(\omega_\beta - \Delta\right)^2} \left(-i(\omega_\beta - \Delta)t + e^{i(\omega_\beta - \Delta)t} - 1\right)\right] + 2\rho_{21}(0)\sum_\beta \frac{|g_\beta|^2}{\omega_\beta^2 - \Delta^2} \left[\cos(\Delta t) - \cos(\omega_\beta t)\right],
\]

where

\[
F_\pm(t) = \sum_\beta \frac{|g_\beta|^2}{\left(\omega_\beta \pm \Delta\right)^2} \sin^2\left(\frac{\omega_\beta \pm \Delta}{2} t\right).
\]

First we analyze the diagonal matrix elements $\rho_{kk}(t)$. For $\Delta << \omega_l$ (for example, in experiment [6] the typical value of $\Delta$ is $10^{10}$ s$^{-1}$, while $\omega_l \approx 5 \cdot 10^{10}$ s$^{-1}$, and $\Delta$ quickly decreases with the interdot distance $d$) we have $F_+(t) \approx B^2(t)/8$, see Eq. (46). As for $F_-(t) = \int_0^\infty d\omega J(\omega) \sin^2[(\omega - \Delta)t/2]/(\omega - \Delta)^2$, one can distinguish two different contributions to this term, one being from the "resonant component", i.e., from the $\delta$-function-like peak of $\sin^2[(\omega - \Delta)t/2]/(\omega - \Delta)^2$ as a function of $\omega$ at $\omega = \Delta$, with a height of $t^2/4$ and a width of $\sim 1/t$, and the other from the remaining "nonresonant background" of the phonon spectrum. Making use of the expression

\[
\frac{\sin^2(\epsilon t)}{\pi t \epsilon^2} \approx \delta(\epsilon),
\]

12
the former can be estimated as $F^{(1)}(t) \approx \Gamma t/4$, where

$$\Gamma = 2\pi \sum_{\beta} |g_{\beta}|^2 \delta(\omega_{\beta} - \Delta) = 2\pi \int_{0}^{\infty} d\omega J(\omega)\delta(\omega - \Delta) = 2\pi J(\Delta) \quad (51)$$

is the rate of the phonon-induced electron transitions $|2\rangle \rightarrow |1\rangle$ (relaxation rate) calculated by the Fermi golden rule [31], and the latter as $F^{(2)}(t) \approx B^2(t)/8$, so that $F(t) \approx \Gamma t/4 + B^2(t)/8$.

Note the different physics behind the two contributions to $F(t)$. While the term $F^{(1)}(t)$ reflects the energy conservation, $\hbar \omega_{\beta} = \Delta$, for a transition $|2\rangle \rightarrow |1\rangle$, the term $F^{(2)}(t)$ arises because of the violation of the energy conservation at short times [31].

Since $\rho_{11}(0) = 1 - \rho_{22}(0)$, one has from Eq. (48):

$$\rho_{11}(t) \approx 1 - \frac{B^2(t)}{2} - \rho_{22}(0) \left[ 1 - \Gamma t - B^2(t) \right] \approx e^{-\frac{\rho_{22}(0)}{2}} - \rho_{22}(0)e^{-\Gamma t - B^2(t)}, \quad (52)$$

where we took into account that $B^2(t) << 1$ at any $t$ and $\Gamma t << 1$ at sufficiently short times (in fact, the standard first-order perturbation theory for calculation of the transition probability is valid at $\Gamma t << 1$, see [31]). This expression for $\rho_{11}(t)$ differs from the commonly used one [20] by the presence of $B^2(t)$ terms which are responsible for the ”non-resonant relaxation” and are time-independent at $t >> \omega_{l}^{-1}$. The ”resonant” term $\Gamma t$ prevails at very short times (note, however, that approximation (50) which leads to the linear dependence of $F^{(1)}$ on $t$ may not hold in this time domain) and, more importantly, at $t > \tilde{t} \approx \Lambda/J(\Delta)$. For $\omega_{d} << \Delta << \omega_{l}$ from Eqs. (17) and (36) one has $\tilde{t} \approx (\omega_{l}/\Delta)^3 \omega_{l}^{-1} \approx 2.5 \cdot 10^{-9} \text{s}$ at $\omega_{l}/\Delta = 5$ and $l = 100 \text{ nm}$.

So, the exponential changes in $\rho_{11}$ and $\rho_{22}$ go into play at $t \approx \tilde{t}$, while at $\omega_{l}^{-1} << t << \tilde{t}$ the diagonal matrix elements are, to the first approximation, time-independent (but different from their initial values), being determined by the value of $\Lambda$.

As for the non-diagonal matrix elements, from Eq. (48) at $\Delta << \omega_{l}$ we have

$$\rho_{12}(t) \approx \rho_{12}(0)e^{i\Delta t}\left[ 1 - 2F_{+}(t) - 2F_{-}(t) \right] + 2\rho_{21}(0)\left[ \Lambda \cos(\Delta t) - \Lambda + \frac{B^2(t)}{4} \right],$$

13
\[ \approx \rho_{12}(0) e^{i \Delta t} \left[ 1 - \frac{B(t)}{2} - \frac{\Gamma t}{2} \right] + 2 \rho_{21}(0) \left[ \Lambda \cos(\Delta t) - \Lambda + \frac{B(t)}{4} \right]. \] (53)

Just like \( \rho_{11}(t) \), along with the usual "resonant" term \( \Gamma t \), this expression contains the "non-resonant" terms \( B(t) \) and \( \Lambda \). At \( \omega_i^{-1} \ll t \ll \tilde{t} \) these terms are greater than the "resonant" one and thus govern the evolution of non-diagonal matrix elements. It is interesting, however, that upon going from the matrix elements \( \rho_{kl} \) in the energy basis \( \{|1\rangle, |2\rangle\} \) to the matrix elements in the basis \( \{|L\rangle, |R\rangle\} \) of localized electron states, the "non-resonant" contributions at \( t \gg \omega_i^{-1} \) can cancel out. For example, if electron initially occupies the left well of the double-well potential, \( |\Psi(0)\rangle = |L\rangle \), i.e., \( \rho_{LL}(0) = 1, \rho_{LR}(0) = \rho_{RL}(0) = \rho_{RR}(0) = 0 \) and hence \( \rho_{11}(0) = \rho_{12}(0) = \rho_{21}(0) = \rho_{22}(0) = 1/2 \), then the probability to find an electron in the right well at time \( t \) is

\[ P_R(t) = \rho_{RR}(t) = \frac{\rho_{11}(t) - \rho_{12}(t) - \rho_{21}(t) + \rho_{22}(t)}{2} \]
\[ = \frac{1}{2} - \text{Re} \rho_{12}(t) \approx \frac{1}{2} \left[ 1 - e^{-\frac{\Gamma t}{2}} \cos(\Delta t) \right]. \] (54)

This simple expression describes the damped electron oscillations between the left and right wells and agrees with that obtained by Wu et al. \[28\].

V. DISCUSSION

Solid-state systems are of great interest in searching for a scalable quantum computer technology, see Refs. \[32, 33\] and references therein. In particular, spatially separated orbital states of an electron in a pair of tunnel-coupled quantum dots \[13, 34, 35\] (or in a singly ionized pair of phosphorous donors in silicon \[26\], etc.) can be used as logical states of a quantum bit (qubit), the logical \( |0\rangle \) (\( |1\rangle \)) being associated with the state \( |L\rangle \) (\( |R\rangle \)) localized in the left (right) double-well potential minimum. These so-called charge qubits can be manipulated, e.g.,
by applying adiabatically switched gate voltages [6, 7, 8, 9, 26] or laser pulses (both resonant and off-resonant) [13, 36, 37, 38, 39] to the system.

The phase gate is realized if the energies $E_L$ and $E_R$ of the states $|L\rangle$ and $|R\rangle$ differ from each other, while electron tunneling between these states is suppressed. Then the qubit vector evolves as $|\Psi(t)\rangle = C_L(t)|L\rangle + C_R(t)|R\rangle = C_L(0)e^{-iE_L t}|L\rangle + C_R(0)e^{-iE_R t}|R\rangle$, the absolute values of $C_L(t)$ and $C_R(t)$ remaining unchanged, and the relative phase $i(E_R - E_L)t$ varying linearly in $t$. This corresponds to the case (i) of strongly asymmetric double-well potential considered above. As follows from the expression (45) for the density matrix, the deformation-phonon-induced qubit decoherence during the phase operation is entirely due to dephasing processes and is quantified by the value of $B^2(t)$, see Eq. (46). At $t >> \omega^{-1}_t$, the value of $B^2(t)$ becomes time-independent and equals to a constant $4\Lambda$, which depends on the material parameters ($\rho, s, \Xi$) and the quantum dot size $l$. For example, this constant is smaller than $10^{-2}$ in the GaAs based quantum dots with $l > 10$ nm, see Eq. (36).

For the amplitude gates, the weights of $|L\rangle$ and $|R\rangle$ states in the qubit state $|\Psi\rangle$ change with time (the combination of the phase and amplitude gates allows for an arbitrary rotation of the qubit vector on the Bloch sphere). For example, $|C_R(T)| = |C_L(0)|$ and $|C_L(T)| = |C_R(0)|$ at operation time $T$ for the quantum NOT. In the absence of decoherence, this gate is implemented at $E_L = E_R$ (i.e., in the case (ii) of symmetric double-well potential) in time $T = \pi\hbar/\Delta \approx 2 \cdot 10^{-10}$ s at $\Delta \approx 10$ meV, see Eq. (54). Decoherence results in the damping of coherent electron oscillations between the dots. At the very early stage of qubit evolution, $t < \omega^{-1}_t = l/s$ (e.g., at $t < 2 \cdot 10^{-11}$ s for the GaAs dot size $l = 100$ nm), both "resonant" and "nonresonant" relaxation processes contribute to the decoherence, see Eq. (53). Contrary to the phase gate, at $t > \omega^{-1}_t$ the decoherence is primarily due to usual "resonant" relaxation [40], and the gate fidelity decreases with time as $1 - 0.5 \exp(-\Gamma t/2)$, see Eq. (54). The value of $\Gamma$ is
extremely sensitive to the system parameters such as the dot size, the interdot distance, etc., see Eqs. (17) and (51). For example, at \( \Delta >> \omega_d \), the decoherence rate \( \Gamma \propto \Delta^3 \exp(-\Delta^2/2\omega_l^2) \) first increases with \( \Delta \) up to the maximum value \( \Gamma_{\text{max}} \) and next decreases rapidly. The value of \( \Gamma_{\text{max}} \) is about \( 5 \cdot 10^9 \text{ s}^{-1} \) in the GaAs dots with \( l = 10 \text{ nm} \) and decreases with \( l \) as \( \Gamma_{\text{max}} \propto l^{-3} \).

At \( \Delta << \omega_d \), the decoherence rate is very small, \( \Gamma \propto \Delta^5 \).

VI. CONCLUSIONS

In this paper, we analized the effect of deformation phonons at the initial stage of coherent electron dynamics in the double-dot structure by the examples of symmetric and strongly asymmetric double-well potential. We have explicitly shown that the phonon-induced decoherence can be due to both dephasing and relaxation (“resonant” and ”nonresonant”) processes, the decoherence rate being determined by the material and double-dot parameters. Making use of the appropriate spectral function \( J(\omega) \), the results obtained can be applied to describe the decoherence due to electron coupling with piezoelectric phonons in the double-dot system [19, 28, 41, 42, 43, 44] and with acoustic phonons in the double-donor Si-based structure [19, 30, 45]. Generalization to the case of nonzero temperature [41, 42, 43, 45] is straightforward. To study the non-Markovian electron dynamics in more detail, it would be interesting to extend the consideration to the longer evolution times through account for \( N \)-phonon states with \( N \geq 2 \).

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