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MATRIX ELEMENTS OF THE DIPOLE-DIPOLE INTERACTION BETWEEN TWO TWO-LEVEL ATOMS DISTANCED ARBITRARILY FROM EACH OTHER

Purpose. As a standard model for describing the processes of a resonant transmission of quantum information on arbitrary distances is the system of two identical two-level atoms, one of which is under radiation of the field of real photons. Such a system can serve as a basis for the construction of an element basis of quantum computers. The purpose of this paper is to study the different modes of dynamics of a system of two identical two-level atoms when they interact with the field of real photons.

Methods. In this paper, we propose a general approach to the description of the processes for the transfer of quantum information from one atom-qubit to another on the arbitrary interatomic distances, which includes two types of new physical effects: the attenuation of quantum states and the retardation of the dipole-dipole interaction.

Results. The optical properties of a system of two identical two-level atoms in collective (symmetric Ψ_s and anti-symmetric Ψ_a) Bell states at arbitrary interatomic distances are investigated. The closed analytical expressions for the shifts and widths of the considered collective states are considered, taking into account the retarded dipole-dipole interaction of atoms. In calculation of the radial matrix elements of the dipole-dipole interaction, the wave functions of the model Fues potential are used.

Conclusions. A detailed study of the mechanisms of resonant transmission of the excitation energy at arbitrary distances between the two-element atoms has an important practical significance for the physical realization of the logical operator CNOT.

Keywords: quantum computer, dipole-dipole interaction, effects of retardation, Fues potential.

Introduction

Search for physical processes performing logical operations is one of the main physical problems associated with the implementation of the idea of the quantum computer and quantum computing [1]. In the papers [2–4], the quantum computer based on electric dipole transitions in a spectrum of two-level atoms interacting selectively with short intensive optical pulses was proposed. As a standard model for describing the processes of a resonant transmission of quantum information at arbitrary distances is the system of two identical two-level atoms, one of which is under radiation of the

field of real photons. Study of various regimes of dynamics of such a model system interacting with the field of real photons can serve as a basis for the construction of an element basis of quantum computers. The theoretically elegant proof of principle possibility of quantum information transmission from one two-level atom to another was given by A.S. Davidov [5], and also by O.N. Gadomsky and K.K. Altunin in aforementioned paper [2].

The problem of two interacting electrons belonging to two different atoms being arbitrarily apart from each other is one of key problems in understanding the processes of resonant transmission of quantum information at arbi-

bitrary distances. A large number of papers (see [2, 6–15] and references therein) are devoted to its study. The main result of these works is that the presence of the second atom can significantly change the lifetime of the excited state of the atom; this change in the lifetime depends on the mutual orientation of the dipole moments of the transition of the atoms and distance between them. Despite existing numerous publications on the resonance interaction of atoms, many aspects of this interaction remain weakly investigated up to this day, especially for two neutral atoms located at an arbitrary distance from each other.

Operator of electric dipole-dipole interaction of two neutral atoms located at an arbitrary distance from each other

The resonance interaction occurs between the excited atom and the atom in the ground state, if the transition energy to the excited state is the same for both atoms (the atoms are in resonance). A similar situation always takes place in the interaction of two identical two-level atoms.

There are several reasons why the theory of resonant interaction of atoms at arbitrary distances from each other deserves further development. First of all, in order to realise experimentally two-qubit quantum operations with cold neutral atoms it is necessary to be able to control the interaction between the qubits [16]. That is why thorough theoretical study of all possible types of atomic interactions is a key to creating a quantum computer with qubits on neutral atoms in optical traps. Depending on the specific quantum states of the atoms involved in the process of quantum information transmission in the system of two qubits, this may be either the Van der Waals interaction or the resonant dipole-dipole interaction each of what is characterized by different dependence on the

interatomic distance R (R^{-6} and R^{-3} respectively, when neglecting the retardation). The dipole-dipole interaction of atoms is stronger in large (relatively to their own sizes) distances, and therefore its use is a priority for increasing the accuracy of quantum operations with neutral atoms.

However, the standard quantum-mechanical calculation of the energy of the resonance interaction of two identical atoms (see, for example, [5]) becomes unsuitable for too large distances of R between them. The fact is that this calculation takes into account only the instantaneous Coulomb interaction of charges (the term $\sim 1/R^3$ in the interaction operator (2) without the retardation factor $\exp(i|\omega_{fi}|R/c)$). Such a consideration is only valid until the interatomic distance R remains small compared with the characteristic wavelengths λ_0 in the spectra of the interacting atoms.

A consistent theory of resonance interaction of atoms that correctly describes the behavior of the forces of the dipole interaction of atoms on both near and far distances can be constructed only if in this theory, all types of atomic electrons interaction that are manifested in different spatial scales are taken into account from the outset. Therefore, in describing the resonance interaction of atoms at arbitrary distances from each other, along with the instantaneous Coulomb interaction, it is necessary to take into account also the retarded interaction of atoms, which depends on the velocity of light c and disappears at $c \rightarrow \infty$.

Such a general consideration was made in [6, 8–11], where the operator $\hat{V}_{LL}^{(\pm)}$ of the retarded interaction of two electrons belonging to two different hydrogen-like atoms at an arbitrary distance from each other. It is convenient to write both parts of the inter-electron interaction operator constructed in [6, 8–11] i.e. the retarded part $\hat{V}_{LL}^{(\pm)}$ and the Coulomb part V_C in the following form:

$$\hat{V}^{(\pm)} = \hat{V}_C + \hat{V}_{LL}^{(\pm)} = \exp\left(\frac{i}{c}|\omega_{fi}^{(1)}|R\right) \left\{ \frac{e^2}{r_{12}} - \frac{e^2}{2m^2c^2} \left[\frac{\hat{p}_1\hat{p}_2 + \vec{n}(\vec{n}\hat{p}_1)\hat{p}_2}{r_{12}} + R^2 \frac{\hat{p}_1\hat{p}_2 - 3\vec{n}(\vec{n}\hat{p}_1)\hat{p}_2}{r_{12}^3} \right] \pm \frac{e^2 R}{2mc} \frac{\vec{n}\hat{p}_1 + \vec{n}\hat{p}_2}{r_{12}^2} \right\}. \quad (1)$$

Here c is the velocity of light, $e = -|e|$ and m are the charge and mass of an electron, $r_{12} = |\vec{r}'_1 - \vec{r}'_2|$ is the distance between electrons belonging to atom 1 and atom 2, $\vec{n} = (\vec{r}'_1 - \vec{r}'_2)/r_{12}$, \vec{r}'_1 and \vec{r}'_2 are the radius-vectors of electrons 1 and 2 in an arbitrary coordinate system, \hat{p}_1 and \hat{p}_2 are the momentum operators of 1-st and 2-nd atomic electrons respectively. In (1) and thereafter, subscripts 1 and 2 differ quantities connected with two different atoms; subscripts i and f characterize the initial and final states of interacting electrons; $|\omega_{fi}^{(j)}| = |\omega_f^{(j)} - \omega_i^{(j)}| \equiv \omega_0$ is the resonant frequency of transition in the spectrum of two-level atoms; $\omega_i^{(j)}$ and $\omega_f^{(j)}$ are the frequencies of initial and final states of j -th electron. In (1), the plus sign in front of the term containing the factor R corresponds to the case $\omega_f^{(1)} > \omega_i^{(1)}$, and the minus sign corresponds to the case $\omega_f^{(1)} < \omega_i^{(1)}$. Oscillating exponential factor (so-called retardation factor) $\exp(i\omega_0 R/c)$ determines the role of time retar-

ation of considered type of atoms interaction [18].

Let the interatomic axis \vec{R} of the diatomic quantum system be directed along the z axis. We will assume further that one two-level atom is at the origin of the coordinate system ($\vec{R}_1 = 0$) and the other at the point \vec{R}_2 with coordinates $(0, 0, R)$. At large distances R , the operator \hat{V}^{\pm} describing the interaction between atoms can be regarded as a small perturbation. Consequently, we can relatively easily estimate the energy of the resonance excitation exchange between two atoms distanced from each other on the basis of the usual perturbation theory. As follows from the derivation (see, for example, [8, 10]) of the formula (1), the operator $\hat{V}^{(\pm)}$ takes into account the transitions in the spectrum of atoms of arbitrary multiplicity. In this paper, we restrict ourselves to considering only electric dipole transitions for which the operator $\hat{V}^{(\pm)}$ is written as:

$$\hat{V}_{dip}^{(\pm)} = \exp\left(\frac{i}{c}\omega_0 R\right) \left\{ \frac{\vec{d}_1\vec{d}_2 - 3(\vec{n}_R\vec{d}_1)(\vec{n}_R\vec{d}_2)}{R^3} \pm \frac{e}{2mc} \left[\frac{\vec{d}_1\hat{p}_2 - 3(\vec{n}_R\vec{d}_1)(\vec{n}_R\hat{p}_2)}{R^2} - \frac{\hat{p}_1\vec{d}_2 - 3(\vec{n}_R\hat{p}_1)(\vec{n}_R\vec{d}_2)}{R^2} \right] - \frac{e^2}{m^2c^2} \frac{\hat{p}_1\hat{p}_2 - (\vec{n}_R\hat{p}_1)(\vec{n}_R\hat{p}_2)}{R} \right\}, \quad (2)$$

where $\vec{n}_R = \vec{R}/R$ is the unit vector in the direction of the inter-atomic axis \vec{R} , $\omega_0 \equiv \omega_{n0} = (E_n - E_0)/\hbar$ is the resonance frequency in the spectrum of two-level atoms, $\vec{d}_1 = e\vec{r}_1$ and $\vec{d}_2 = e\vec{r}_2$ are the operators of the electric dipole moments of separate atoms, \vec{r}_1 and \vec{r}_2 are the radius-vectors of electrons 1 and 2 relatively nuclei of atoms $A(1)$ and $A(2)$, respectively. This operator is known as the generalized operator of electric dipole-dipole interaction of two neutral atoms located at an arbitrary distance from each other.

The energy of resonance interaction of atoms at arbitrary distances

Let us consider the system of two identical atoms at an arbitrary distance R from each other. In each atom, we will be interested in the transition between the same pair of levels, and the other levels will not manifest themselves in the considered process of resonant transfer of the excitation energy from one atom to another. In fact, in nature, there are practically no atomic systems with only two energy levels. But if

the interaction with the field is of pronounced resonant character, then, as a rule, the influence of other levels can be neglected. Thus, the two-level atom represents a certain mathematical model of qubit – a carrier of quantum information. The existence in the atomic quantum system of two selected internal basis states and the principle of superposition is enough to store one bit of quantum information – a qubit. We characterize each atom-qubit with two levels of energy E_0 and E_n having the resonant transition frequency $\omega_0 = \omega_{fi}^{(1)} = -\omega_{fi}^{(2)} = (E_n - E_0)/\hbar$ and the wave functions $\varphi_0(j)$ and $\varphi_n(j)$. The subscripts 0 and n denote the ground and excited states of the atom, respectively, and the argument $j = (1, 2)$ of the wave function indicates a number of the electron (and a number of the atom) to which it belongs.

Classical computers operate with bistable transistor circuits that have a nonlinear relationship between the input and output voltages [1]. In a quantum computer, a role of such a bistable transistor circuit plays a two-level atom having two orthogonal states $|0\rangle$ and $|n\rangle$, between which an electric single-electron dipole transition with a resonant frequency ω_0 is allowed. Let the state $|0\rangle$ with the wave function $\varphi_0(j)$ and the energy E_0 be a logical “0” $\equiv |0\rangle$ and the state $|n\rangle$ with the wave function $\varphi_n(j)$ and the energy E_n ($E_n > E_0$) be a logical “1” $\equiv |n\rangle$. The level-to-level dipole transitions $|0\rangle \leftrightarrow |n\rangle$, $E_0 \leftrightarrow E_n$ with the matrix element of the dipole moment of atom transition $(\vec{d}_j)_{n0} = \langle n|\vec{d}_j|0\rangle$ correspond to the transitions “0” \leftrightarrow “1”. As noted in [1], a quantum bistable element (qubit) has a new (compared with the classical one) property of the superposition of states: it can be in any superposition state $|\varphi\rangle = \alpha|0\rangle + \beta|n\rangle$, where α and β are complex numbers satisfying the condition $|\alpha|^2 + |\beta|^2 = 1$. It is the quantum principle of states superposi-

tion that allows the quantum computer to provide fundamentally new possibilities.

For the system of two interacting atoms having only one electron, the Hamiltonian \hat{H} can be represented in the form of sum of Hamiltonians of isolated atoms, $\hat{H}_0 = \hat{H}_1(\vec{r}_1) + \hat{H}_2(\vec{r}_2)$, and operator of electric dipole-dipole interaction between them, $\hat{V}_{dip}^{(\pm)}$:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V}_{dip}^{(\pm)} \\ &= \hat{H}_1(\vec{r}_1) + \hat{H}_2(\vec{r}_2) + \hat{V}_{dip}^{(\pm)}(\vec{r}_1, \vec{r}_2; R). \end{aligned} \quad (3)$$

Let $E_{n_1 n_2} = E_{n_1} + E_{n_2}$ and $|n_1 n_2\rangle$ are respectively the eigenvalue and eigenfunction of operator of energy $\hat{H}_0 = \hat{H}_1 + \hat{H}_2$ without interatomic interaction. In accordance with the partition (3), let us denote the wave function of the state of the system in which both the non-interacting atoms are in the ground state by $|00\rangle$, that is,

$$\begin{aligned} |00\rangle &= \varphi_0(1)\varphi_0(2) \exp(-iE_0 t_1/\hbar) \\ &\times \exp(-iE_0 t_2/\hbar) \equiv \tilde{\varphi}_0(1)\tilde{\varphi}_0(2). \end{aligned} \quad (4)$$

Here E_0 is the energy of the initial states of the first $A(1)$ and second $A(2)$ atoms, the numbers 1 and 2 correspond to the coordinates and times for the atoms $A(1)$ and $A(2)$, respectively. For neutral atoms having not constant dipole moments, the energy correction to the two-atom system is equal to zero, because $\langle 00|\hat{V}_{dip}^{(\pm)}|00\rangle = 0$. At the same time, the dipole-dipole interaction being effective at small distances between atoms distorts in some way the wave functions of atomic states. Thus, in the first approximation of the perturbation theory in the interatomic interaction $\hat{V}_{dip}^{(\pm)}$ (2), the perturbed wave function of the system of two identical atoms in the ground state is of the standard form (see, for example, [5, 17]):

$$\Psi_0(1)\Psi_0(2) = \tilde{\varphi}_0(1)\tilde{\varphi}_0(2) + \sum_{n_1 n_2} \frac{\langle \tilde{\varphi}_{n_1}(1)\tilde{\varphi}_{n_2}(2)|\hat{V}_{dip}^{(\pm)}|\tilde{\varphi}_0(1)\tilde{\varphi}_0(2)\rangle}{2E_0 - E_{n_1} - E_{n_2}} \tilde{\varphi}_{n_1}(1)\tilde{\varphi}_{n_2}(2), \quad (5)$$

where summation is carried out with respect to all possible intermediate states of atoms except of $|00\rangle$. According to the representation (5),

a non-zero correction to the energy of the two neutral atoms system in the ground state will appear only in the second order of the pertur-

bation theory [5, 17, 18]. We consider the state $\Psi_0(1)\Psi_0(2)$ (see (5)) as an initial state of pair of atoms interacting with field of real photons.

Let the final state $|n0\rangle$ of two resonant atoms corresponds to the excited state $|n\rangle$ of atom $A(1)$ with wave function $\tilde{\varphi}_n(1) = \varphi_n(1) \exp(-iE_n t_1/\hbar)$ and energy E_n as well as the ground state $|0\rangle$ of atom $A(2)$ with wave function $\tilde{\varphi}_0(2) = \varphi_0(2) \exp(-iE_0 t_2/\hbar)$ and energy E_0 . According to the resonance condition, the state $|0n\rangle$ being described by the wave function $\tilde{\varphi}_0(1)\tilde{\varphi}_n(2)$ corresponds to the same energy. Consequently, the unperturbed system (two isolated identical atoms) has the additional degeneration here associated with the possibility of permutation of states between atoms. In the first approximation of the perturbation theory, we have the energy matrix of the second order. It is diagonalized when constructing symmetric and antisymmetric linear combinations of the initial wave functions of individual atoms:

$$\Phi_s(1, 2) = \frac{1}{\sqrt{2}} [\tilde{\varphi}_n(1)\tilde{\varphi}_0(2) + \tilde{\varphi}_0(1)\tilde{\varphi}_n(2)], \quad (6)$$

$$\Phi_a(1, 2) = \frac{1}{\sqrt{2}} [\tilde{\varphi}_n(1)\tilde{\varphi}_0(2) - \tilde{\varphi}_0(1)\tilde{\varphi}_n(2)]. \quad (7)$$

In the case of complex atoms $A(1)$ and $A(2)$ with an arbitrary number of electrons, the interaction between them at small distances R plays a significant role. In this, the Hamiltonians \hat{H}_1 and \hat{H}_2 as well as the zeroth approximation functions Φ_s (6) and Φ_a (7) should be interpreted in the approximation of the self-consistent field for the two-center potential [19]. In this case, \hat{V}_{dip}^\pm is the correlation interaction of atoms with each other. The transition to the corresponding operator of the electric dipole-dipole interaction \hat{V}_{dip}^\pm of atoms with many electrons can be carried out by transition in (2) from the momentum operator $v\hat{e}cp_j$ of j -th electron to the operator of the dipole moment \vec{d}_j [5] and the subsequent replacement of the operators \vec{d}_1 and \vec{d}_2 by the operators of the dipole moments of the atoms $A(1)$ and $A(2)$, respectively.

In order to obtain corrections to the energy of symmetrical (6) and antisymmetrical (7) states of the system of two resonant atoms in the first order of perturbation theory one has to cal-

culate the mean values of the perturbation operator \hat{V}_{dip}^\pm (2) in these states, i.e.,

$$\begin{aligned} \Delta E_s &= \langle \Phi_s | \hat{V}_{dip}^\pm | \Phi_s \rangle, \\ \Delta E_a &= \langle \Phi_a | \hat{V}_{dip}^\pm | \Phi_a \rangle. \end{aligned} \quad (8)$$

Substituting the expressions (2), (6) and (7) into (8), after simple transformations with use of the known ratio [5]

$$\langle n | \hat{p}_j | 0 \rangle = i \frac{m\omega_0}{e} \langle n | \vec{d}_j | 0 \rangle$$

we obtain the final expression

$$\begin{aligned} \Delta E_s(R) &= -\Delta E_a(R) = \omega_0^3 e^{i\omega_0 R/c} |\langle n | \vec{d} | 0 \rangle|^2 \\ &\times \left[\left(\frac{1}{\omega_0^3 R^3} - \frac{i}{c\omega_0^2 R^2} \right) \Phi(1, 2) - \frac{\Phi'(1, 2)}{c^2 \omega_0 R} \right] \\ &\equiv \Delta E_{AA}(R). \end{aligned} \quad (9)$$

Here

$$\begin{aligned} \Phi(1, 2) &\equiv \cos \theta_1^x \cos \theta_2^x + \cos \theta_1^y \cos \theta_2^y \\ &\quad - 2 \cos \theta_1^z \cos \theta_2^z, \\ \Phi'(1, 2) &\equiv \cos \theta_1^x \cos \theta_2^x + \cos \theta_1^y \cos \theta_2^y \end{aligned}$$

are the geometric factors depending on the orientation of dipole transitions in both atoms, θ_i^x , θ_i^y , θ_i^z ($i = 1, 2$) are the angles between one of corresponding axes and the direction of dipole transition in i -th atom $A(i)$. When writing the expression (9) it is taken into account that the atom-qubits of the considered quantum system are identical, that is, they have identical matrix elements of the operator of the dipole moment between the ground $|0\rangle$ and excited $|n\rangle$ states:

$$|\langle n | \vec{d}_1 | 0 \rangle| = |\langle n | \vec{d}_2 | 0 \rangle| = |\langle n | \vec{d} | 0 \rangle| \equiv |(\vec{d})_{n0}|.$$

Note that the quantity ΔE_s (ΔE_a) is complex shift of energy E_s (E_a) of symmetrical (antisymmetrical) state Φ_s (Φ_a) of the pair of identical atoms. For further analysis, in the formulas (9) for ΔE_s and ΔE_a , it is convenient to separate explicitly real and imaginary parts:

$$\Delta E_s = \delta E_s - \frac{i}{2} \hbar \gamma_s, \quad \Delta E_a = \delta E_a - \frac{i}{2} \hbar \gamma_a. \quad (10)$$

The complexity of the shifts ΔE_s and ΔE_a reflects in the first place purely relativistic effects of retardation of the interaction (1) of two resonant atoms at an arbitrary distance from each other. The appearance of imaginary terms

$-i\hbar\gamma_s/2$ and $-i\hbar\gamma_a/2$ in $\Delta E_{s(a)}$ (10) arising from the retarded dipole-dipole interaction of atoms, was first revealed in [20], and later, independently in the more systematic approach [14].

The first-order corrections to the energy $E_n + E_0$ of initially degenerated collective states (6) and (7) give only real parts δE_s and δE_a of the complex shifts (8):

$$\begin{aligned} \delta E_{s,a}(R) &= \pm \text{Re} \Delta E_{AA}(R) \\ &= \pm e^2 |\langle n | \vec{r} | 0 \rangle|^2 F(1, 2; R). \end{aligned} \quad (11)$$

The dependence of the shifts $\delta E_{s(a)}(R)$ on the interatomic distance R is completely determined by the multiplier $F(1, 2; R)$. In order to simplify the expression (11), there is the notation used:

$$\begin{aligned} F(1, 2; R) &= \\ &= \left[\frac{\Phi(1, 2)}{R^3} - \frac{\omega_0^2 \Phi'(1, 2)}{c^2 R} \right] \cos \left(\frac{\omega_0 R}{c} \right) \\ &+ \frac{\omega_0 \Phi(1, 2)}{c R^2} \sin \left(\frac{\omega_0 R}{c} \right), \end{aligned} \quad (12)$$

where the plus and minus signs in (11) correspond to the symmetric Φ_s and the antisymmetric Φ_a wave functions of the pair of identical atoms. As can be seen in (11), for the states of different symmetries (Φ_s (6) and Φ_a (7)) with respect to permutations of atoms, the considered retarded dipole-dipole interaction gives the shifts δE_s and δE_a having opposite signs: $\delta E_s = -\delta E_a$. At the same time, with increasing R moduli of the shifts $\delta E_{s(a)}$ of energy levels of the system of dipole-dipole interacting atoms decrease and tend to zero in the limit of separated ($R \rightarrow \infty$) atoms as $1/R$.

Let us study the behavior of $\delta E_{s(a)}(R)$ in the limiting cases of large and small R . Thus, the expressions for δE_s and δE_a can be essentially simplified at $\omega_0 R/c \rightarrow 0$, when linear sizes of two-atom quantum system are much smaller than characteristic wave length $\lambda_0 = 2\pi c/\omega_0$ in spectrum of interacting atoms ($R \ll \lambda_0$). In this limiting case, one can neglect the retardation of the dipole-dipole interaction of atoms, that makes it possible to substitute $\cos(\omega_0 R/c) = 1$, $\sin(\omega_0 R/c) = \omega_0 R/c$ in the expression (12) for $F(1, 2; R)$ and to omit terms proportional to $1/R$ and $1/R^2$. Then, instead of

(11) we obtain

$$\delta E'_{s,a} = \pm \frac{e^2}{R^3} |\langle n | \vec{r} | 0 \rangle|^2 \Phi(1, 2). \quad (13)$$

As it is expected, this expression coincides with the known formula [5] for the energy of resonant exchange of excitations between two neutral atoms located closely from each other.

We now consider the opposite limiting case $\omega_0 R/c \gg 1$, when the distance between atoms is much larger than the wavelength $\lambda_0 = 2\pi c/\omega_0$. As can be seen from (1) and (2), only the mostly long-range retardation term, proportional to $1/R$, plays the main role in the interaction between atoms (when $R \gg \lambda_0$). For this reason, in the formula (12) for the factor $F(1, 2; R)$, terms decreasing with the distance as $1/R^2$ and $1/R^3$ can be neglected. As a result, for sufficiently large R ($R \geq 0$), the expression (11) got the following form:

$$\begin{aligned} \delta E_s &= -\delta E_a = \\ &= -\frac{e^2 \omega_0^2 \Phi'(1, 2)}{c^2 R} |\langle n | \vec{r} | 0 \rangle|^2 \cos \left(\frac{\omega_0 R}{c} \right). \end{aligned} \quad (14)$$

This expression is consistent with the corresponding formula [20] for the energy of the resonance excitation exchange between two distant ($R \gg \lambda_0$) neutral atoms.

Let us take note of the following important circumstance related to the difference between formulas (11) and (13). The presence of the real $\cos(\omega_0 R/c)$ and imaginary $\sin(\omega_0 R/c)$ parts of the retardation factor $\exp(i\omega_0 R/c)$ in various terms of the expression (12) indicates to the complicated periodic dependence of the matrix element of the excitation transfer $\delta E_{s(a)}(R)$ on the interatomic distance R . It is this property of the oscillating behavior of $\delta E_{s,a}(R)$ on the background of power decreasing ($\sim 1/R$) with the distance R being slower than (13) is the most characteristic feature of the formula (11) for the energy of the resonant excitation exchange between two neutral atoms. The dependence of $\delta E_{s,a}(R)$ on R distinguishes from (13) due to the retardation part of the dipole-dipole interaction of atoms.

Therefore, we see that at account of dipole-dipole interatomic interaction (2) the symmetrical and antisymmetrical states of the

pair of atoms have the different energies

$$\begin{aligned} E_s &= E_n + E_0 + \delta E_s \\ &= E_n + E_0 + e^2 |\langle n | \vec{r} | 0 \rangle|^2 F(1, 2; R), \end{aligned} \quad (15)$$

$$\begin{aligned} E_a &= E_n + E_0 + \delta E_a \\ &= E_n + E_0 - e^2 |\langle n | \vec{r} | 0 \rangle|^2 F(1, 2; R). \end{aligned} \quad (16)$$

Two collective states of the system of two resonant atoms: symmetric s and antisymmetric a , initially degenerated with respect to energy, are described by the two types of wave functions Φ_s (6) and Φ_a (7) which with taking into account the corrections $\delta E_s, \delta E_a$ to the energy $E_n + E_0$ can be written as

$$\begin{aligned} \Psi_s &= \Phi_s \exp(-i\delta E_s t_1 / \hbar), \\ \Psi_a &= \Phi_a \exp(-i\delta E_a t_1 / \hbar), \end{aligned} \quad (17)$$

where Φ_s and Φ_a are determined in (6) and (7), t_1 is the local time for the atomic pair associated with the position of the atom $A(1)$.

As can be seen from (15) and (16), the dipole-dipole interaction between atoms leads to the splitting of the initially degenerate (with respect to the energy) level $E_0 + E_n$ into two collective energy levels E_s (15) and E_a (16) distanced from each other by the quantity $\Delta E = E_s - E_a = 2\delta E_s$, which characterizes the process of resonance transfer of the excitation energy from one atom to another. At the same time, due to the resonance interaction of atoms, the energy level E_s (15) lies $\Delta E = 2\delta E_s$ above the level E_a (16).

Thus, in order to calculate the energy of symmetric E_s (15) and antisymmetric E_a (16) states of the system of two resonant atoms, it is necessary to calculate the matrix elements of the dipole transitions $\langle n | \vec{r} | 0 \rangle$. In this case, the wave function should take into account the influence of the electrons of the atomic core on the non-Coulomb additive to the potential acting on the valence electron in the atom.

$$\langle r | nlj \rangle = \frac{2Z_i^{3/2}}{\nu_{nl}^2} \sqrt{\frac{(2\lambda + 2)_{n_r}}{n_r! \Gamma(2\lambda + 2)}} \left(\frac{2Z_i r}{\nu_{nl}} \right)^\lambda \exp\left(-\frac{Z_i r}{\nu_{nl}}\right) {}_1F_1\left(-n_r; 2\lambda + 2; \frac{2Z_i r}{\nu_{nl}}\right); \quad (20)$$

Here, the standard notations for the gamma function $\Gamma(x)$ and the Pochhammer symbol $(a)_n = a \cdot (a+1) \cdot \dots \cdot (a+n-1)$ [23] are used. It is obvious that this solution satisfies the standard requirements of continuity, uniqueness and boundedness in the entire numerical semiaxis,

Such a modification is present, for example, in the Fues model potential, which takes into account simultaneously action of the polarization potential on states with large orbital quantum numbers l and the action of the Pauli principle that “forces out” a valence electron from the core in states with small l [21]. The Fues potential for the motion of an electron in the field of an ion residue with the charge Z_i has the form

$$V(r) = -\frac{Z_i}{r} + \sum_l \frac{B_l(E)}{r^2} \hat{P}_l, \quad (18)$$

where \hat{P}_l is the projection operator on the subspace of states with the orbital moment l , $B_l(E)$ is the constant that changes the centrifugal potential in this subspace in such a way that the eigenvalues $E_{nl} = -Z^2 / (2\nu_{nl}^2)$ of the corresponding radial Schrödinger equation, which are determined by the effective principal quantum number [21, 22]

$$\begin{aligned} \nu_{nl} &= n_r + \lambda_{nl} + 1, \\ \lambda_{nl} &= \sqrt{(l + 1/2)^2 + 2B_l(E_{nl})} - 1/2 \end{aligned} \quad (19)$$

(λ is the effective orbital moment, $n_r = 0, 1, 2, \dots$ is the radial quantum number), coincide exactly with energies of a real atom.

The eigenfunctions of the radial Hamiltonian with the potential (18) normalized by the condition

$$\int_0^\infty |\langle r | nlj \rangle|^2 r^2 dr = 1$$

can be written using the confluent hypergeometric function ${}_1F_1(a; c; x)$ in the form

which represents the distance from the atomic nucleus to electron $r \in [0; \infty)$. Therefore, after integrating, the radial matrix element $R_{nn'}$ in (15) and (16) can be represented analytically using the generalized hypergeometric function of two variables F_2 [23, 24]:

$$R_{nn'} = \frac{1}{4Z_i} \frac{\Gamma(\lambda + \lambda' + 4)}{\sqrt{\Gamma(2\lambda + 2)\Gamma(2\lambda' + 2)}} \sqrt{\frac{(2\lambda + 2)_{n_r}}{n_r!} \frac{(2\lambda' + 2)_{n'_r}}{n'_r!}} \left(\frac{2\nu}{\nu + \nu'}\right)^{\lambda_l + 2} \left(\frac{2\nu'}{\nu + \nu'}\right)^{\lambda_l + 2} \times \\ \times F_2\left(\lambda + \lambda' + 4; -n_r; -n'_r; 2\lambda + 2; 2\lambda' + 2; \frac{2\nu'}{\nu + \nu'}, \frac{2\nu}{\nu + \nu'}\right), \quad (21)$$

where the primed quantities refer to the final state, and non-primed ones – to the initial state.

Summary

In this paper, on the basis of the theory of resonance interaction of atoms through the field of virtual photons [6, 8–11], the influence of the retarded dipole-dipole interaction of atoms on the formation and decay of quasi-stationary collective (symmetric Ψ_s and antisymmetric Ψ_a) states of the quantum system consisting of two

fixed identical two-level atoms is investigated. The closed analytic expressions for the shifts and widths of the considered collective states Ψ_s and Ψ_a are obtained taking into account the retarded dipole-dipole interaction of atoms. The theoretical analysis of the shift and splitting of the collective energy levels of the given system caused by interatomic interaction is carried out. The asymptotic expansions of the real and imaginary parts of energy of the quasi-stationary Bell states Ψ_s and Ψ_a in the limit of large and small interatomic distances are studied.

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МАТРИЧНЫЕ ЭЛЕМЕНТЫ ДИПОЛЬ-ДИПОЛЬНОГО ВЗАИМОДЕЙСТВИЯ МЕЖДУ ДВУМЯ ДВУХУРОВНЕВЫМИ АТОМАМИ, РАСПОЛОЖЕННЫМИ НА ПРОИЗВОЛЬНОМ РАССТОЯНИИ ДРУГ ОТ ДРУГА

Исследовано оптические свойства системы из двух одинаковых двухуровневых атомов в коллективных (симметричном Ψ_s и антисимметричного Ψ_a) белловских состояниях при произвольных межатомных расстояниях. Получены замкнутые аналитические выражения для сдвигов и ширин рассматриваемых коллективных состояний с учетом запизнюющей диполь-дипольного взаимодействия атомов. При исчислении радиальных матричных элементов диполь-дипольного взаимодействия использованы волновые функции модельного потенциала Фьюса.

Ключевые слова: квантовый компьютер, диполь-дипольное взаимодействие, эффекты запаздывания, потенциал Фьюса.

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МАТРИЧНІ ЕЛЕМЕНТИ ДИПОЛЬ-ДИПОЛЬНОЇ ВЗАЄМОДІЇ МІЖ ДВОМА ДВОРІВНЕВИМИ АТОМАМИ, РОЗТАШОВАНИМИ НА ДОВІЛЬНІЙ ВІДСТАНІ ОДИН ВІД ОДНОГО

Досліджено оптичні властивості системи з двох однакових дворівневих атомів у колективних (симетричному Ψ_s і антисиметричному Ψ_a) беллівських станах при довільних міжатомних відстанях. Отримано замкнуті аналітичні вирази для зсувів і ширин розглядуваних колективних станів з урахуванням запізнюючої диполь-дипольної взаємодії атомів. При обчисленні радіальних матричних елементів диполь-дипольної взаємодії використано хвильові функції модельного потенціалу Фьюса.

Ключові слова: квантовий комп'ютер, диполь-дипольна взаємодія, ефекти запізнювання, потенціал Фьюса.

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