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High-Frequency Properties of Double-Well Nanostructures

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Abstract—On the basis of analytical and numerical solutions of the Schrödinger equation, the active polarization current and emission efficiency of double-well nanostructures were calculated in a wide range of amplitudes of alternating electromagnetic field. It is shown that generation in the important terahertz region with smooth frequency tuning and the highest efficiency are possible. The behavior of the coefficient of reflection of electrons from the structure is studied; this coefficient goes to zero under the conditions of maximum efficiency.

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1. INTRODUCTION

In [1–3], we studied the generation of electromagnetic radiation in a double-well nanostructure (DWNS). A double-well nanostructure consists of two tunneling-connected quantum wells (QWs) to which a constant voltage V_{dc} is applied. An analytical theory was developed for the structure's model with δ-shaped barriers. It was shown that it is possible to generate electromagnetic radiation in the important terahertz range with gradual tuning of frequency and efficiency close to the highest available. However, the guaranteed region of application is limited by comparatively small amplitudes of the electromagnetic field.

In this study, we use numerical methods to calculate the active current and emission efficiency in a wide range of high fields. In addition, we determined the coefficient of electron reflection from a DWNS. The calculations were performed for two types of interaction of electrons with an electromagnetic field. The results of both types of interactions coincide with each other with good accuracy.

2. FORMULATION OF THE PROBLEM. BASIC EQUATIONS

Let us consider a one-dimensional (1D) structure with δ-function barriers at the points $x = 0$, a, and $2a$; the structure consists of two QWs (Fig. 1). A dc electric field with the potential V_{dc} is applied to the second QW in the DWNS. On the left ($x \longrightarrow -\infty$), a steady-state electron flux is supplied to the first QW; this flux is characterized by the quantity q^2 and an energy ε that is approximately equal to the energy of the resonance level $\varepsilon_R^{(1)}$ in the first QW. An ac electric field $E(t) = E_0\cos\omega t$ is in effect in the structure region.

The electron wave function $\Psi(x, t)$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi}{\partial x^2} + \alpha\sum_{n=0}^{2}\delta(x-na)\Psi - V_{dc}\Theta(x-a)\Psi - \hat{V}\Psi, \quad (1)$$

where α is the barrier strength, Θ is the unit-step function, m^* is the effective electron mass in the structure, and $\hat{V}$ is the operator of interaction of an ac electric field E with electrons (this operator can be of two types). The $\hat{V}$ operator of the first type is defined as

$$\hat{V} = \frac{1}{2m^*}\left(2\frac{e\hbar}{c}iA(t)\frac{\partial}{\partial x} + \frac{e^2}{c^2}A^2\right), \quad (2)$$

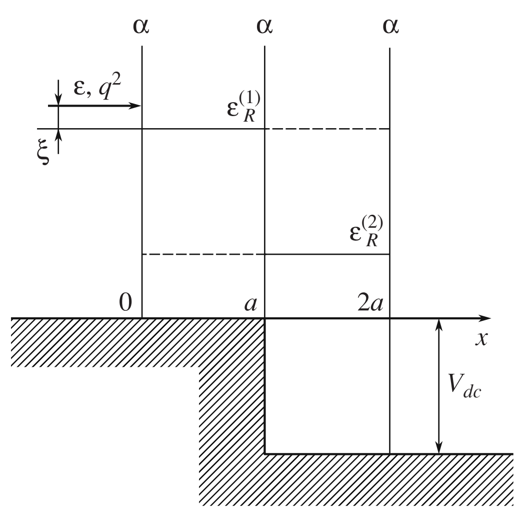

Fig. 1. A double-well nanostructure with voltage applied. The strength of δ-function barriers α = 10; the width of the wells $a = 2\pi$.

where $A = -cE_0(\sin\omega t)/\omega$ is the vector potential in Coulomb calibration ($\partial A/\partial x = 0$), while the expression for the second type of operator is written as

$$\hat{V} = eE_0 x\cos\omega t. \qquad (3)$$

In what follows, we assume that $\hbar = 2m^* = c = 1$ for convenience. We write the boundary conditions for the Schrödinger equation (1) as [3]

$$\begin{cases} \Psi(0,t)\left(1-\dfrac{\alpha}{ip}\right)+\dfrac{1}{ip}\dfrac{\partial\Psi(0,t)}{\partial x} = 2q\exp\left(-\dfrac{i\varepsilon t}{\hbar}\right), \\ \Psi(2a,t)\left(1-\dfrac{\alpha}{ip_1}\right)-\dfrac{1}{ip_1}\dfrac{\partial\Psi(2a,t)}{\partial x} = 0, \end{cases} \qquad (4)$$

where $p = \sqrt{\varepsilon}$ and $p_1 = \sqrt{\varepsilon + V_{dc}}$ are the wave numbers of an electron on the left and on the right of the structure, respectively.

The reduced current of the nth well J_n is defined by the following expression:

$$J_n(t) = \frac{2}{a}\int_{a(n-1)}^{an} dx\,\mathrm{Im}\left\{\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}\right\}, \qquad (5)$$
$$n = 1, 2.$$

Under the effect of an ac electric field, active (i.e., in-phase with the external field) J_c and reactive J_s polarization currents appear in the structure. The in-phase current in the nth well is expressed as

$$J_{cn} = \frac{\omega}{\pi}\int_0^{2\pi/\omega} dt J_n(t)\cos(\omega t), \quad n = 1, 2; \qquad (6)$$

it is important that $J_{c1} \approx J_{c2} = J_c$ (see [2]). A detailed description of numerical and analytical methods for determining J_c in low and high ac fields was given in [1–3]. In our calculations, we chose a structure with the barrier strength $\alpha = 10$ and wells with the width $a = 2\pi$ ($\alpha/p \approx \alpha a/\pi = 2\alpha = 20$).

3. RESULTS OF THE ANALYTICAL THEORY

An analytical theory of coherent resonance tunneling in a double-well nanostructure in the presence of an ac electromagnetic field and a dc electric field was developed in [1, 2]. It is shown that the energy spectrum of the structure consists of two levels $\varepsilon_R^{(1)}$ and $\varepsilon_R^{(2)}$ appearing due to interference between the wells. The resonance frequency of the electromagnetic field is assumed to be equal to the difference between energies of these levels: $\varepsilon_R^{(1)} - \varepsilon_R^{(2)} = \omega$.

The most important quantity is the active current of the first well (equal to the current of the second well) [2]

$$J_c = -\frac{EQ\Gamma^2\eta}{|\Delta(\lambda)|^2}, \quad \eta = \frac{e^2p^2}{\alpha}\left[\frac{V_0+\sqrt{1+V_0^2}}{1+V_0^2}\right], \qquad (7)$$

$$|\Delta(\lambda)|^2 \approx [(\bar{\lambda}^2+\Gamma^2-\xi^2)^2+4\Gamma^2\xi^2],$$

$$\bar{\lambda} = \frac{\lambda}{\sqrt{1+V_0^2}} = \frac{V_{ac}}{8\sqrt{1+V_0^2}},$$

$$V_0 = V_{dc}/t_0, \quad t_0 = \frac{4p_0^2}{\alpha a}, \qquad (8)$$

$$\Gamma = \frac{2p_0^3}{\alpha^2 a}, \quad p_0 = \frac{\pi}{a} = \frac{1}{2}, \quad Q = pq^2.$$

Here, $\xi = \varepsilon - \varepsilon_R^{(1)}$, t_0 is the splitting energy, V_{ac} is the ac electric potential, Γ is the width of the levels, and Q is the amplitude of electron flux. The active current J_c gives rise to amplification and generation of an electromagnetic field (see [1, 2]). In order to analyze the efficiency of generation, we use the measure of efficiency $\tilde{P}$ introduced previously by us [2]

$$\tilde{P} = \frac{1}{2pq^2}\left[\frac{1}{2\pi}\int_0^{2\pi/\omega} dt\int_0^{2a} dx J_{1c}(x,t)E(t)\right]$$
$$= \frac{2\lambda^2\Gamma^2[V_0+\sqrt{1+V_0^2}]}{|\Delta(\lambda)|^2[1+V_0^2]^{3/2}}. \qquad (9)$$

The efficiency $\tilde{P}$ is equal to the ratio between the number of photons emitted by DWNS in the unit time and the number electrons supplied to a DWNS using resonance tunneling. Expressions (7)–(9) were obtained in [2] under the assumption that the following quantity is small:

$$\tilde{V}^2 = \frac{\lambda^2}{4\Gamma^2(1+V_0^2)} = \frac{V_{ac}^2}{256\Gamma^2(1+V_0^2)}. \qquad (10)$$

It can be easily seen that the guaranteed region of applicability of (7)–(9) is not wide, especially at small values of V_0. Therefore, it is of interest to calculate the active current and efficiency in a wide range of high fields and, in particular, determine the true limits of applicability of expressions (7)–(9).

4. THE CURRENT AND EFFICIENCY OF EMISSION FROM A DOUBLE-WELL NANOSTRUCTURE IN THE CASE OF A LOW ELECTROMAGNETIC FIELD

At first, we study the current J_c and efficiency $\tilde{P}$ in a low field, in which case $\bar{\lambda} \ll \Gamma$. The Schrödinger equation (1) was solved with the interaction potentials $\hat{V}$ of both types. Similar results were obtained, as was predicted in the previous analytical study [2]. In Fig. 2, we show the results of calculations of the dependence of the current $\tilde{J}_c = -J_c/2eEa$ on the frequency ω at various values of the dc voltage V_{dc}. It can be seen that $\tilde{J}_c$ features sharp maxima at the resonance frequencies ω_m; these frequencies coincide with the energy difference between the resonance levels $\varepsilon_R^{(1)}$ and $\varepsilon_R^{(2)}$ [1]:

$$\omega_m = t_0\sqrt{1+V_0^2}. \quad (11)$$

The value of the current at the maximum is specified by (7) if we assume that $\bar{\lambda} \ll \Gamma$:

$$\tilde{J}_c = \tilde{J}_c(0)\frac{V_0+\sqrt{1+V_0^2}}{1+V_0^2}, \quad (12)$$

where $\tilde{J}_c(0) = \tilde{J}_c(V_0 = 0)$. Let us compare the dependence (12) of $\tilde{J}_c$ on $V_0 = V_{dc}/t_0$ with the results of numerical solution. We can easily obtain from (12) that the current increases with increasing voltage V_{dc} and attains a maximum at

$$V_{dc}^m = \frac{t_0}{\sqrt{3}} \approx 23\Gamma, \quad (13)$$

which is consistent with the run of the curve and the position of the maximum in Fig. 2.

The efficiency in a low field at $\xi = 0$ is equal to

$$\tilde{P} = \frac{2\lambda^2[V_0+\sqrt{1+V_0^2}]}{\Gamma^2[1+V_0^2]^{3/2}}. \quad (14)$$

We can see that $\tilde{P}$ is a small quantity proportional to λ^2/Γ^2. As the voltage V_0 increases ($V_0 \gg 1$) the efficiency rapidly decreases according to the law $1/V_0^2$. Thus, the efficiency of a DWNS in a low field is very low.

5. EFFICIENCY OF EMISSION OF DOUBLE-WELL NANOSTRUCTURES IN HIGH ELECTROMAGNETIC FIELDS

It was shown analytically in [2] that there exists a basic possibility of radically increasing the efficiency $\tilde{P}$ to the highest possible value, i.e., to unity. This efficiency is attained under optimal conditions, in which case the energy of supplied electrons ξ and the field $\bar{\lambda}$ satisfy the following equations:

$$\xi = \xi_0 = \pm\sqrt{\bar{\lambda}^2-\Gamma^2}, \quad \bar{\lambda} > \Gamma, \quad \frac{V_{ac}}{8\Gamma} > \sqrt{1+V_0^2}. \quad (15)$$

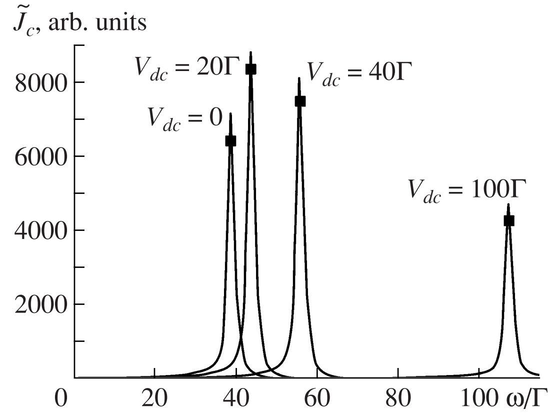

Fig. 2. Dependence of the active current $\tilde{J}_c$ on the frequency of alternating field ω at several values of the voltage V_{dc}: the solid line represents the numerical result, while the points correspond to the result of analytical calculation.

Equations (15) are obtained from requirements for a maximum in $\tilde{P}$ (9) with respect to ξ. Introducing ξ_0 into (9), we obtain the efficiency of emission in the peaks as

$$\tilde{P}_m = \frac{1}{2}\frac{[V_0+\sqrt{1+V_0^2}]}{\sqrt{1+V_0^2}}. \quad (16)$$

If $V_0 = 0$, $\tilde{P}(0) = 1/2$; at $V_0 \gg 1$, the highest attainable efficiency $\tilde{P}_m(\infty) = 1$ is realized. This means that each electron supplied to a DWNS emits a photon. If $\bar{\lambda} < \Gamma$, there is a single maximum in the efficiency at $\xi = 0$ and $\tilde{P}_m(0) < 1$. Thus, the behavior of DWNS in an ac field is similar to the behavior of two-level coherent laser based on the single-well structure [4].

The results of numerical solution are shown in Fig. 3, where the dependence of the efficiency $\tilde{P}$ on the ξ tuning for different values of V_{ac} at large values of V_{dc} is $V_{dc} = 100\Gamma$ ($V_0^2 = 6.25 \gg 1$). It can be seen from Fig. 3, that, at $V_{ac}/\Gamma = 20$, there exists a single maximum at $\xi_0 = 0$. At $V_{ac}/\Gamma = 40$ and 80, two maxima appear for the positive and negative adjustments of ξ_0; the amplitudes of these maxima increase as the amplitude of the voltage V_{ac} increases. The value of efficiency at the peaks is close to unity.

In Fig. 3, we also show the analytical dependences $\tilde{P}(\xi)$, which are in good agreement with the numerical dependences. Some asymmetry in the numerical results is also consistent with analytical calculation if this asymmetry is taken into account according to [2]. The

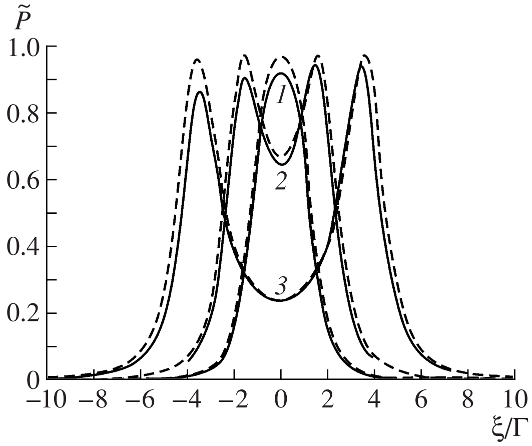

Fig. 3. Dependences of the emission efficiency for a double-well nanostructure $\tilde{P}$ on tuning ξ for several values of alternating-field potential V_{ac} in the case of $V_{dc} = 100\Gamma$: the solid lines represent the results of numerical calculations, while dashed lines represent the results of analytical calculations; V_{ac} = (*1*) 20Γ, (*2*) 40Γ, and (*3*) 80Γ.

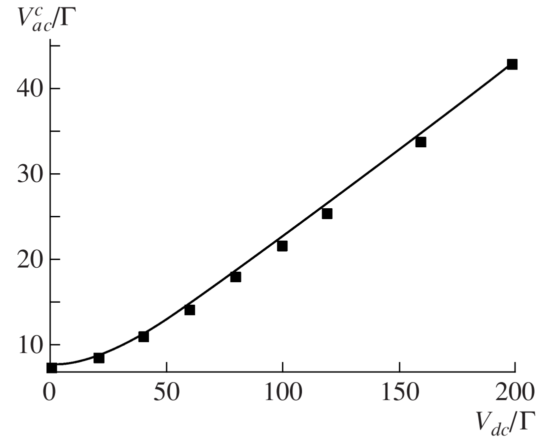

Fig. 4. Dependence of the critical field V_{ac}^c (at which two maxima in the efficiency $\tilde{P}$ appear) on the voltage V_{dc}: the solid line represents the results of analytical calculations, while squares represent the results of numerical calculations.

point is that we dropped (for simplicity) small terms that disturb symmetry in formulas (7) and (8).

Let us now compare critical values V_{ac}^c of the field at which optimal conditions are attained according to (15). In Fig. 4, we compare (15) with numerical results. It can be seen that there is excellent agreement between the analytical and numerical results. In particular, we have the critical value $V_{ac}^c/\Gamma \approx 22$ at $V_{dc}/\Gamma = 100$. The rates of shift of maxima of the efficiency $\xi_0(\bar{\lambda})$ are shown in Fig. 5. Again, the analytical value of ξ_0 obtained using formula (15) is in good agreement with the results of numerical calculations.

Thus, we may state that the formulas of analytical theory [2] describe adequately the qualitative and quantitative behavior of efficiency, until $V_{ac}/\Gamma = 80$. In this case, the small parameter of the theory $\tilde{V}^2$ becomes larger than unity ($\tilde{V}^2 \approx 3$); i.e., the range of applicability is found to be wider than $\tilde{V}^2 < 1$.

We now report the results of numerical calculations for the opposite case: $V_{dc} = 0$. The dependence $\tilde{P}(\xi)$ is shown in Fig. 6. If the value of V_{ac} is smaller than the critical value ($V_{ac}^c/\Gamma = 8$), there is a single maximum at $\xi_0 = 0$ (see the curve at $V_{ac}/\Gamma = 1$); then, we have a bimodal dependence at $V_{ac} = 20$ or 40. The efficiency at the maxima $\tilde{P}_m$ does not exceed 1/2. Agreement with the analytical results is quite good; however, this agreement is worse than in the case of $V_{ac}/\Gamma = 100$ (as expected), so that $\tilde{V}^2 \approx 6$ at $V_{ac}/\Gamma = 40$. The rate of motion of maxima of efficiency and critical value V_{ac}^c become equal to each other (see Fig. 5) and indicate that the analytical and numerical results agree with high accuracy.

In conclusion, we note that numerical calculations were performed for both types of interaction of electrons with an electromagnetic field (see formulas (2) and (3)). The results coincide with each other with high accuracy.

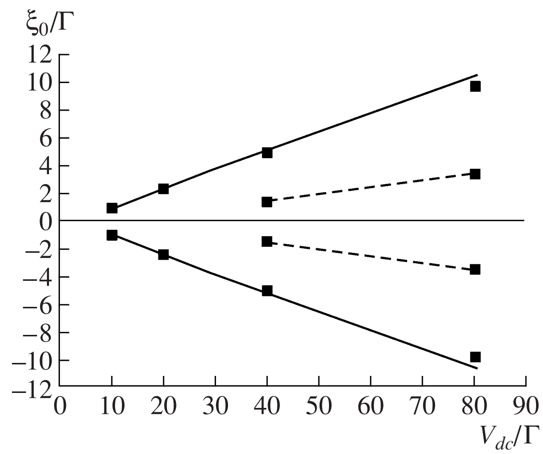

Fig. 5. Dependences of the magnitudes of tuning ξ_0 (at which the efficiency features a maximum $\tilde{P}_m$) on the alternating-field potential V_{ac}: the lines represent the results of analytical calculations for $V_{dc} = 0$ (the solid line) and $V_{dc} = 100\Gamma$ (dashed lines); squares represent the results of numerical calculations.

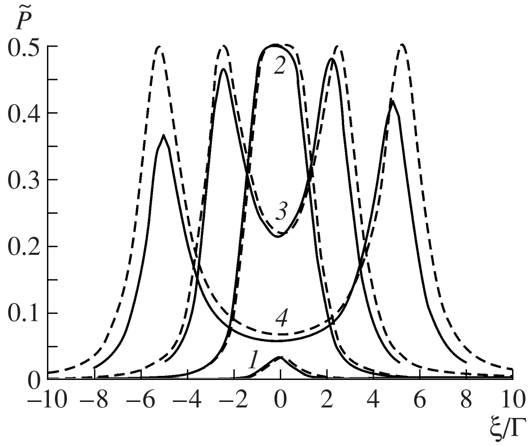

Fig. 6. Dependences of the emission efficiency $\tilde{P}$ for a double-well nanostructure on tuning ξ at several values of the alternating-field potential V_{ac} in the case of V_{dc} = 0: the solid lines represent the results of numerical calculation, while dashed lines represent the results of analytical calculations. V_{ac} = (*1*) Γ, (*2*) 8Γ, (*3*) 20Γ, and (*4*) 40Γ.

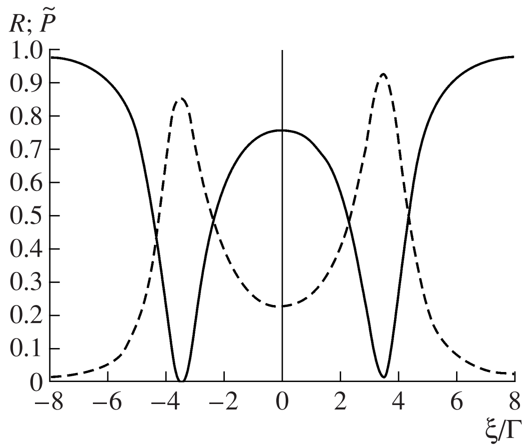

Fig. 7. Dependences of the reflection coefficient R (the solid line) and the emission efficiency of the double-well nanostructure $\tilde{P}$ (dashed line) on the tuning ξ at V_{ac} = 80Γ and V_{dc} = 100Γ.

6. COEFFICIENTS OF REFLECTION AND TRANSMISSION FOR A DOUBLE-WELL NANOSTRUCTURE IN A HIGH ELECTROMAGNETIC FIELD

As was shown analytically [2] and confirmed by the data in Section 5, the behavior of a DWNS is similar to the behavior of a coherent laser based on a QW [4]; in this laser, radiative transitions occur between resonance levels in the QW. At the same time, it has been shown [4] that the reflection coefficient R goes to zero (consequently, the transmission coefficient T becomes equal to unity) under optimal conditions. Therefore, we should expect that the R and T coefficients of a DWNS feature similar properties. By definition [4], the reflection coefficient

$$R = \frac{|\psi_1(0) - q|^2}{q^2}$$

is expressed in terms of the wave function of the upper level $\psi_1(0)$ as

$$\psi_1(x) = \frac{\omega}{2\pi}\int_0^{2\pi/\omega} dt\Psi(x,t)\exp(i\varepsilon t). \quad (17)$$

In Fig. 7, we show the dependences of the reflection coefficient on the tuning ξ at V_{dc} = 100Γ and V_{ac} = 80Γ. For the sake of comparison, we present the emission efficiency $\tilde{P}$. It can be seen that the maxima of efficiency correspond to the minima of reflectance (to maxima in transmittance); it is noteworthy that reflectance in the case of optimal tuning ξ_0 is close to zero. Thus, reflection from a DWNS behaves as reflection in a coherent laser, which confirms the similarity of DWNS and this laser.

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