Influence of non-linear electrons interaction at their transport through the symmetric two- barrier resonance nano-system

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The quantum mechanical theory of permeability coefficient and negative active conductivity of mono-energetic electronic flux through the plane symmetric two-barrier resonance tunnel structure which can be an active element of quantum cascade laser is developed within the models of effective masses and rectangular potentials taking into account the electron-electron interaction. The properties of permeability coefficient and conductivity as functions of electrons energies and frequency of electromagnetic radiation are established. It is shown how the properties of active conductivity can be used for the experimental evaluation of resonance energies and widths of working electron quasi-stationary states.

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1. Introduction

The theory of electronic transport through the twobarrier resonance tunnel structures (RTS), fig. 1, is important in particular, because these nano-systems are used as an active elements of quantum cascade lasers (QCL) operating in the actual range of electromagnetic waves frequencies – the windows of atmosphere transparency. The main physical characteristics: intensity of laser radiation, excited current and so on essentially depends just on the properties of negative active conductivity.

In the prevailing number of papers [1-5] concerning the theory of physical processes in QCL, the transport properties of electronic currents through the RTS are studied. However, the electron-electron interaction is not considered, as a rule, due to the mathematical problems of the solution of non-linear differential equations.



Fig. 1. Energy scheme for the electrons and geometry of two-barrier RTS.

In our paper the theory of active negative conductivity and permeability coefficient for the open two-barrier RTS is developed. The electron-electron interaction and their interaction with electromagnetic field are taken into account within the models of rectangular potential barriers and different quasi-particle effective masses in wells and barriers of RTS.

The problem of non-linear electron-electron interaction in physics of bosons and quasi-particles in some other models is studied in a lot of papers [6-11]. However, the developed mathematical methods can not be directly used for the research of electronic transport through the open RTS.

The similar problem was observed in papers [12, 13]. The rectangular potential barriers were approximated by δ -like ones in order to avoid the mathematical difficulties. The known fault of simplified model [14] is automatic ignoring of different electron effective mass in RTS wells and barriers. It brings to the overestimated magnitudes of resonance energies of electron quasi-stationary states (QSS) at tens per cents and resonance widths – tens times over.

2. Hamiltonian of the system. Permeability coefficient and active conductivity for symmetric two-barrier RTS

The plane open symmetric two-barrier RTS, fig. 1, is studied in Cartesian coordinate system with OZ axis perpendicular to the nano-system planes. The small difference of lattice constants for layers-wells and layersbarriers allows to use the model of effective masses and rectangular potentials, where:

$$m(z) = m_0 \sum_{p=0}^{2} (\theta(z - z_{2p-1}) - \theta(z - z_{2p})) + m_1 \sum_{p=0}^{1} [\theta(z - z_{2p}) - \theta(z - z_{2p+1})],$$
(1)

$$U(z) = U \sum_{p=0}^{1} \left[\theta(z - z_{2p}) - \theta(z - z_{2p+1}) \right] \quad . \tag{2}$$

Here $\theta(z) = \begin{cases} 0, z < 0, \\ 1, z \ge 0 \end{cases}$ Heaviside step function;

 $z_{-1} = -\infty, \ z_4 = \infty$.

It is assumed that mono-energetic electronic beam is falling at RTS from the left side, perpendicularly to its planes. The electrons are characterized by the energy E, density of current $j_0^+ \sim \sqrt{E}$ and concentration n_0 . The electronic current is considered one-dimensional and complete Schrodinger equation is written as:

$$i\hbar \frac{\partial \Psi(E,z,t)}{\partial t} = [H(E,z) + H(z,t)]\Psi(E,z,t).$$
(3)

Here

$$H(E,z) = -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} + U(z) + \upsilon |\Psi(E,z)|^2 \quad (4)$$

– the Hamiltonian of quasi-stationary case (expression of Gross-Pitaevsky type) containing the energy $(v|\Psi(E,z)|^2)$ of non-linear electron-electron interaction in Hartree-Fock approximation where $\Psi(E,z)$ function satisfies the equation:

$$H(E,z)\Psi(E,z) = E \Psi(E,z).$$
⁽⁵⁾

The Hamiltonian of electron interaction with varying in time electromagnetic field characterized by frequency ω and not big intensity of electric field C allows assume it small in the frames of perturbation theory. Thus, it can be written in convenient analytical calibration (not Coulomb one):

$$H(z,t) = H(z)(e^{i\omega t} + e^{-i\omega t}), \qquad (6)$$

where

$$H(z) = -eC\{z[\theta(z) - \theta(z - z_3)] + z_3\theta(z - z_3)\}.$$

The equation (3) has not the exact solution, since, taking into account H(z, t), it can be solved in the so-called approximation of weak signal when $\Psi(E,z,t)$ wave function is taken as:

$$\Psi(E, z, t) = \Psi(E, z)e^{-i\omega_0 t} + \Psi_1(E, z, t), \ (\omega_0 = E \hbar^{-1}), \ (7)$$

where $\Psi(E,z)$ satisfies equation (5) and the correction of the first order to the wave function in one-mode approximation is:

$$\Psi_{1}(E,z,t) = \Psi_{+1}(E,z)e^{-i(\omega_{0}+\omega)t} + \Psi_{-1}(E,z)e^{-i(\omega_{0}-\omega)t}.$$
 (8)

Preserving the first order magnitudes in equation (3) and considering (7), (8), the system of two non-linear equations is obtained for $\Psi_{\pm 1}(E,z)$ functions:

$$[H(E,z) - \hbar(\omega_0 \pm \omega)]\Psi_{\pm 1}(E,z) + H(z)\Psi(E,z) = 0.$$
(9)

In order to solve it, we have to find the analytical expression for $\Psi(E,z)$ function which is the solution of non-linear Schrodinger equation (5). As far as two-barrier RTS is an open one, this equation is solved taking into account the conditions of wave function and its density of current continuity at all interfaces ($\eta \rightarrow +0$):

$$\Psi(E,z)\Big|_{z=z_p-\eta} = \Psi(E,z)\Big|_{z=z_p+\eta} \quad (p=0,1,2,3)$$

$$\frac{1}{m(z)} \frac{\partial \Psi(E,z)}{\partial z}\Big|_{z=z_p-\eta} = \frac{1}{m(z)} \frac{\partial \Psi(E,z)}{\partial z}\Big|_{z=z_p+\eta}$$
(10)

together with the normality condition:

$$\int_{-\infty}^{\infty} \Psi^*(k',z)\Psi(k,z) = \delta(k-k') \quad (11)$$

$$(k = \hbar^{-1}\sqrt{2m_0E})$$

Now, $\Psi(E,z)$ wave function is obtained within two methods: numeric Monte-Carlo and recursive one.

Monte-Carlo method is well known but the calculation of $\Psi(E,z)$ wave function at the strong electronelectron interaction demands unacceptable amount of time. Consequently, further we use this method calculating the wave functions for the particular systems with respectively not big non-linearity. The results almost exactly coincide to the ones obtained by recursive method. The latter allows obtain the wave functions for equation (5) quickly and with demanded exactness even for the big magnitudes of non-linear electron-electron interaction.

The solution of non-linear equation (5) within recursive method is performed in such a way. First of all we solve the linear Schrodinger equation (without interaction):

$$H_0 \Psi_0(E, z) = E \Psi_0(E, z).$$
 (12)

Its exact solution is known:

$$\Psi_0(E,z) = \tag{13}$$

$$\begin{split} &= \sum_{p=1}^{3} (A_{p}(E)e^{ik_{p}z} + B_{p}(E)e^{-ik_{p}z}) \Big[\theta(z - z_{p-1}) - \theta(z - z_{p}) \Big] + \\ &+ (A_{0}(E)e^{ik_{0}z} + B_{0}(E)e^{-ik_{p}z}) \theta(-z) + A_{4}(E)e^{ik_{0}z} \theta(z - z_{3}), \end{split}$$

where geometric parameters of two-barrier RTS are:

$$z_0 = 0;$$
 $z_1 = \Delta;$ $z_2 = b + \Delta;$ $z_3 = b + 2\Delta.$ (14)

The magnitudes k_p are determined by the dynamic characteristics of electron:

$$k_0 = k_2 = k_4 = k = \hbar^{-1} \sqrt{2m_0 E};$$

$$k_1 = k_3 = \hbar^{-1} \sqrt{2m_1 (U - E)}$$
(15)

and $A_p(E)$, $B_p(E)$, $B_0(E)$, $A_4(E)$ coefficients are definitely fixed by $A_0(E)$ coefficient, in its turn related to the density of current, falling at two-barrier RTS: $j_0^+ = en_0 \sqrt{2Em_0^{-1}} |A_0(E)|^2$.

The equation (5) can not be directly solved using $\Psi_0(E,z)$ function, expr. (13). But the known now $|\Psi_0(E,z)|^2$ function can be expressed as a sum of *N* piece-continuous functions:

$$|\Psi_0(E,z)|^2 =$$
 (16)

$$= \lim_{N \to \infty} \sum_{p=0}^{N} |\Psi_0(E, z_{2p})|^2 [\theta(z - z_{2p-1}) - \theta(z - z_{2p+1})],$$

where

$$z_p = \frac{p}{2N}b;$$
 $z_{-1} = z_0 = 0;$ $z_{2N} = z_{2N+1} = b + 2\Delta.$

Its example, as function of E and z is shown in fig. 2a.

Now then, for the rather big magnitudes N >>1, the continuous function $|\Psi_0(E,z)|^2$ can be replaced by piececontinuous function $|\widetilde{\Psi}_0(E,z)|^2 \approx |\Psi_{0N}(E,z)|^2$ with demanded exactness. According to this, the non-linear potential $(\upsilon|\Psi_0(E,z)|^2)$ transits into piece-continuous one $(\upsilon|\widetilde{\Psi}_0(E,z)|^2)$ in equation (5). Using the latter, we can solve the equation (5) together with the continuity conditions (10) and find $\Psi_1(E,z)$ non-linear function in the first approximation of perturbation theory.

Using $\Psi_{I}(E,z)$ function we find $|\Psi_{I}(E,z)|^{2}$ in the form of piece-continuous functions (at *N*>>1):

$$\left| \widetilde{\Psi}_{I}(z, E) \right|^{2} = \lim_{N \leftarrow \infty} \sum_{p=0}^{N} \left| \Psi_{I}(z_{2p}, E) \right|^{2} [\theta(z - z_{2p-1}) - \theta(z - z_{2p+1})].$$
(17)

Substituted into (5) together with conditions (10), $\left|\widetilde{\Psi}_{I}(E,z)\right|^{2}$ function makes the potential linear in the intervals corresponding to z variable. It, again, allows solve the Schrodinger equation and obtain the wave function $\Psi_{II}(E,z)$ in second cycle (approximation).

Within the recursive method $\Psi(E,z)$ function as the solution of non-linear equation (5) in arbitrary S cycle can be found:

$$\Psi(E,z) = \Psi_{\mathcal{S}}(E,z). \tag{18}$$

The number of cycles (S), used for $\Psi(E,z)$ recursive calculation, is determined be the desired exactness and is controlled by the evident condition:

$$\zeta = \max_{E,z} \left\{ \frac{\left| \Psi_{S}(E,z) \right|^{2} - \left| \Psi_{S-1}(E,z) \right|^{2}}{\left| \Psi_{S}(E,z) \right|^{2}} \right\} <<1.$$
(19)

It is clear that the fixed exactness (ζ) for $\Psi(E,z)$ calculation depends on the magnitude of potential of electron-electron interaction (v): the bigger it is, the bigger number of cycles (S) one has to perform.

The example of $|\Psi(E,z)|^2$ dependence on *E* and z in the vicinity of the energies of two first electron QSSs at different magnitudes of potential of electron-electron interaction (v) is shown in fig. 2b. Fig. 2 proves that the results obtained within both methods: Monte-Carlo (a) and recursive (b), are almost coinciding and the difference between them is not observed.

The obtained wave function (18), according to quantum mechanics [15], allows obtain the permeability coefficient:

$$D(E) = \left| A_0(E) \right|^{-2} \cdot \operatorname{Im} \left\{ \Psi(E, z) \frac{\partial \Psi(E, z)}{k \, \partial z} \right\}_{z=z_3 + \eta}$$
(20)

for the electronic current through the two-barrier RTS. It is known from refs. [14, 15] that using the permeability coefficient D(E) one can obtain the spectral parameters (resonance energies and resonance widths) of electron QSSs. The positions of D(E) maxima in energy scale define the resonance energies (E_n) and their widths at the half of the height define the resonance widths (Γ_n) of *n*-th QSS. The analysis of D(E) properties for the two-barrier RTS, experimentally investigated [16-19], is performed in the next section.



Fig. 2. Evolution of $|\Psi(E,z)|^2$ function for two first electron QSSs (n = 1, 2): a) v=0 (n = 1, 2); b) $v=10^{-3}$ meV (n=1), v=0.1 meV (n=2) for the two-barrier RTS with geometric parameters: $\Delta=2.1$ nm, b=10.8 nm

The obtained $\Psi(E,z)$ wave function allows to take the solutions of non-linear equations (9) as:

$$\Psi_{\pm 1}(E,z) = \Psi_{\pm}(E,z) + \Phi_{\pm}(E,z), \qquad (21)$$

where $\Psi_{\pm}(E,z)$ – the solutions of homogeneous, $\Phi_{\pm}(E,z)$ – exact partial solutions of heterogeneous equations (9).

The solutions of homogeneous equatios (9) are written as:

 $\Psi_+(E,z) =$

$$\sum_{p=0}^{4} \left[B_{\pm}^{(p)}(E) e^{-ik_{\pm}^{(p)}(z-z_{p-1})} + A_{\pm}^{(p)}(E) e^{ik_{\pm}^{(p)}(z-z_{p-1})} \right] \times \left[\theta(z-z_{p-1}) - \theta(z-z_{p}) \right], \quad \left(A_{\pm}^{(0)} = B_{\pm}^{(4)} = 0 \right) \quad (22)$$

where

$$k_{\pm}^{(0)} = k_{\pm}^{(2)} = k_{\pm}^{(4)} = \sqrt{2m_0(E \pm \hbar\omega)/\hbar^2}, \qquad (23)$$

$$k_{\pm}^{(1)} = k_{\pm}^{(3)} = \sqrt{2m_1((E - U) \pm \hbar\omega)/\hbar^2}.$$

The partial solutions of heterogeneous equations (9) are known:

$$\Phi_{\pm}(E,z) = \sum_{p=0}^{3} \left[\mp \frac{e\mathcal{C}}{\hbar\omega} z \Psi_{0}^{(p)}(E,z) + \frac{e\mathcal{C}}{m_{p}(z)\omega^{2}} \frac{d\Psi_{0}^{(p)}(E,z)}{dz} \right] \times \left[\theta(z-z_{p-1}) - \theta(z-z_{p}) \right] \mp \frac{e\mathcal{C}}{\hbar\omega} z_{3} \Psi_{0}^{(4)}(z_{3},E) \theta(z-z_{3}) \cdot (24)$$

The conditions of wave functions (21) and their densities of currents continuity at all nano-system interfaces bring to the system of eight heterogeneous equations fixing eight coefficients $(B_{\pm}^{(0)}(E), A_{\pm}^{(4)}(E))$,

 $B^{(p)}_{\pm}(E), A^{(p)}_{\pm}(E), p=0.3$).

Finally, we have obtained the function $\Psi_{\pm}(E,z)$, correction of the first order $\Psi_1(E,z,t)$ and, thus, the complete wave function $\Psi(E,z,t)$.

The complete wave function of electrons interacting with periodic in time electromagnetic field, according to quantum mechanics, determines the density of electronic current through the nanostructure:

$$j(E,z,t) = \frac{ie\hbar n_0}{2m(z)} \left[\Psi(E,z,t) \frac{\partial}{\partial z} \Psi^*(E,z,t) - \Psi^*(E,z,t) \frac{\partial}{\partial z} \Psi(E,z,t) \right].$$
(25)

Taking into account the small sizes of two-barrier RTS compared to the electromagnetic wave length, in quasi-classic approximation for the quantum transitions accompanied by radiation, further we perform the calculation of guided current defining the absolute value of negative active conductivity:

$$\sigma(E,\omega) = \left|\sigma^{+}(E,\omega) + \sigma^{-}(E,\omega)\right|, \quad (26)$$

where

$$\sigma^{+}(\omega) = \frac{\hbar^{2} \omega n_{0}}{2m_{0} z_{3} C^{2}} \left(k_{+}^{(4)} \left| A_{+}^{(4)}(E) \right|^{2} - k_{-}^{(4)} \left| A_{-}^{(4)}(E) \right|^{2} \right),$$

$$\sigma^{-}(\omega) = \frac{\hbar^{2} \omega n_{0}}{2m_{0} z_{3} C^{2}} \left(k_{+}^{(0)} \left| B_{+}^{(0)}(E) \right|^{2} - k_{-}^{(0)} \left| B_{-}^{(0)}(E) \right|^{2} \right).$$
(27)

Here $\sigma^+(E,\omega)$, $\sigma^-(E,\omega)$ – the partial terms of conductivity caused by the electronic currents interacting with electromagnetic field and flowing forward ($\sigma^+(E,\omega)$) and backward ($\sigma^-(E,\omega)$) respectively the starting current falling at two-barrier RTS.

3. Influence of non-linear electron-electron interaction at the conductivity and permeability of two-barrier RTS

Influence of electron-electron interaction at the conductivity and permeability of open two-barrier RTS is

studied for the plane nano-structure consisting of $In_{0.53}Ga_{0.47}As$ – wells and $In_{0.52}Al_{0.48}As$ – barriers and physical parameters: $m_0=0.046 m_e$, $m_1=0.089 m_e$, U=516 meV.

In fig. 2 the dependence of $|\Psi(E,z)|^2$ on energy (*E*) and coordinate (*z*) is presented in the vicinity of the energies of two first electron QSSs for the different magnitudes of electron-electron interaction (υ) in order to explain the changes of permeability coefficient $D(E, \upsilon)$ and active conductivity $\sigma(E, \omega, \upsilon)$. Figure proves that independently on υ magnitude, $|\Psi(E,z)|^2$ function at E=const has *n* maxima in the vicinity of *n*-th QSS, the same as in the case of closed nanostructure. At fixed magnitude of coordinate, $|\Psi(E,z=const)|^2$ as function of energy more and more deflects from Lorentz shape and is deformed in such a way that its high-energy wing rapidly decays while the lowenergy one, gradually raising, becomes more sloping.

The clarified properties of $|\Psi(E,z)|^2$ determine the evolution of permeability coefficient $D(E, \upsilon)$ shape depending on energy (*E*) in the vicinity of first and second QSS for the different magnitudes of electron-electron interaction (υ), fig. 3. At this figure, the evolution of $D(E, \upsilon)$ in δ -barrier model is presented for the comparison for the same two-barrier RTS.

It is known that δ -barrier model overestimates the resonance energies of electron QSSs at tens percents and the resonance widths ten times over, comparing to the model of rectangular potentials. It is clear from fig.3 that the electron-electron interaction in realistic model causes the essential deformation of permeability coefficient even when the interaction is two orders smaller than δ -barrier model gives.

Fig. 3 also proves that at v=0 the evolution of D(E, v)qualitatively equal for the both models. The is permeability coefficient for all QSSs has the shape of Lorentz curve with maximal value $D(E_n, \nu)=1$ at all resonance energies E_n with resonance widths Γ_n . At the increasing of electron-electron interaction energy, the shape of $D(E, \nu)$ in the vicinity of renormalized resonance energies $(E_n(v))$ at first becomes quasi-Lorentz. At further v increasing, the function D(E, v) is more and more deformed: its low-energy wing is slowly raising in the vicinity of maximum, obtaining quasi-Lorentz dependence on E and high-energy wing sharply, almost plumb, decays. Thus, in the vicinity of resonance energies $(E_n(v))$ renormalized by interaction, the shape of D(E, v) very differs from the Lorentz one and becomes wedge-like for the rather big v magnitudes.

Consequently, now it is necessary to generalize the sense of resonance energies $(E_n(\upsilon))$ and widths $(\Gamma_n(\upsilon))$ characterizing the symmetric Lorentz curve so that they would be extended at the wedge-like shape of $D(E, \upsilon)$. The way of the procedure is clear from fig. 4. Really, the generalization of resonance energies $(E_n(\upsilon))$ is evident. The generalized resonance width $(\Gamma_n(\upsilon))$ of *n*-th QSS is convenient to introduce as a sum of low-energy $(\gamma_{nl}(\upsilon))$ and high-energy $((\gamma_{nh}(\upsilon))$ widths because, since $\gamma_{nl}(\upsilon \rightarrow 0) = \gamma_{nh}(\upsilon \rightarrow 0) = \Gamma_n(0)/2$, then quite such procedure ensures the correct limit case $\Gamma_n(\upsilon \rightarrow 0) = \Gamma_n$.



Fig. 3. Dependences of permeability coefficient D on energy E in the vicinity of two first electron QSSs at different magnitudes of electron-electron interaction energy v obtained within the model of rectangular potentials (a), δ -barrier model (b) for two-barrier RTS with geometrical parameters Δ =2.4 nm, b=21.6 nm.

Fig. 4 proves the expediency and convenience of using the generalized resonance energies and widths as generalized spectral parameters of permeability coefficient $D(E, \upsilon)$. At the figure one can see the dependence of generalized resonance energy on the magnitude of electron-electron interaction $(E_n(\upsilon))$ and generalized resonance width $(\Gamma_n(\upsilon))$ – within the distance between the curves $E_n(\upsilon)+\gamma_{nh}(\upsilon)$ and $E_n(\upsilon)-\gamma_{nl}(\upsilon)$.

The dependence of conductivity $\sigma(E,\omega,v)$ on the energy of electromagnetic field ($\hbar\omega$) at v=0; $5\cdot10^{-5}$ meV for the several electron energies (*E*) in the range E_2 - $\Gamma_2/2 \le E \le E_2 + \Gamma_2/2$ is shown in fig. 5 for the two-barrier RTS with geometric parameters $\Delta=2.4$ nm, b=21.6 nm (left and down scales). The permeability coefficient as function of electron energy (right and up scales) is presented in the vicinity of generalized resonance energy of the second QSS (central figure) and in the



Fig. 4. Dependences of generalized resonance energies and widths of two electron QSSs (n=1, 2) on energy of electron-electron interaction (υ) at Δ =2.1 nm and b = 10.8 nm

vicinity of the first QSS (insert figure) for the same υ magnitudes.

Fig. 5 proves that independently of υ magnitude, the permeability coefficient $D(E, \upsilon)$ in the vicinity of generalized resonance energy of second electron QSS almost coincides with normalized enveloping over the energy function:

$$\widetilde{\sigma}(E,\omega,\upsilon) =$$

$$=\sigma(E,\omega,\upsilon)/\sigma(E_2(\upsilon),(E_2(\upsilon)-E_1(\upsilon))\hbar^{-1},\upsilon)$$

The difference between both functions is not visible at the figure. In the vicinity of the generalized resonance energy of the first electron QSS, the function D(E, v) almost coincides with normalized active conductivity:

$$\widetilde{\sigma}(E_2, \omega, \upsilon) =$$
$$= \sigma(E, \omega, \upsilon) / \sigma(E_2(\upsilon), \omega, \upsilon)$$

From the figure one can also see that the electronelectron interaction almost does not influence at the maximal magnitude of conductivity $\sigma(E,\omega)$. However, the function $\sigma(E,\omega,\upsilon)$ is weakly shifted, proportionally to the interaction energy ($\upsilon \max |\Psi(E,z)|^2$), into the region of smaller frequencies. Its shape is deformed from Lorentzlike to wedge-like.



Fig. 5. Active conductivity (σ) as function of electromagnetic field energy ($\hbar\omega$) at different energies (E), left and down scales, respectively. Permeability coefficient (D) as function of energy (E), right and up scales, respectively. Dotted curves: v=0; solid curves: $v=5\cdot10^5$ meV

4. Conclusions

The quantum mechanical theory of electrons active conductivity is developed for the open two-barrier RTS taking into account the electron-electron interaction. It is established that the electron-electron interaction almost does not influence at the maximal intensity of electromagnetic radiation, proportional to the absolute value of negative active conductivity maximum ($\sim \max \sigma(E, \omega)$). The whole $\sigma(E, \omega)$ function is weakly shifted into low-energy region and its shape changes from Loretz-like to wedge-like.

Experimentally scanning the active conductivity for the two-barrier RTS by mono-energetic electronic beam, one can obtain σ as function of energy (*E*) and frequency (ω). It would allow the evaluating of spectral parameters: generalized resonance energies and widths of working QSSs of electron.

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