Self-consistent analytic solution of the Schrödinger equation for resonant interaction between electrons and an hf electric field in double-barrier structures

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A self-consistent analytic time-dependent solution of the Schrödinger and Poisson equations describing interaction between electrons and an hf electric field in double-barrier structures has been obtained. The time-dependent space-charge density limits the transition probability between neighboring levels and suppresses transitions in which the level number changes by more than unity. The smaller the level number, the stronger the effect of the dynamic space charge.
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The search for self-consistent solutions of the Schrödinger and Poisson equations remain one of most interesting problems of quantum mechanics. But even in the static case, which can be treated using well-developed techniques (for aplications involving double-barrier resonant tunneling structures, see Refs. 1–3), solutions are usually obtained numerically. This paper reports on a problem in which self-consistent solutions of time-dependent Schrödinger and Poisson equations can be obtained analytically. This is the problem of resonant interaction between an electron in a symmetric double-barrier structure and hf electric field, and it is interesting not only from the standpoint of pure science, but also for its practical significance, because this interaction is the driving force in semiconductor generators of coherent radiation, and such generators operating in the terahertz range have been studied extensively in recent years.

Consider the transport of a monoenergetic flux of electrons across a simple double-barrier symmetric structure of width a with thin (δ-like) barriers[4,5] and no dc electric field. A weak potential which is a harmonic function of time is applied to the structure, and the space charge and electric field outside the device are zero. The effect of static space charge is ignored (one can assume, for example, that this charge is cancelled by ionized donors). Let the uniform electric field inside the structure vary in time as $E(t)=E(e^{i\omega t}+e^{-i\omega t})$. For definiteness, we assume that electrons move from left to right. Then under these assumptions, the time-dependent Schrödinger equation has the form

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2}+\alpha\delta(x)\psi+\alpha\delta(x-a)\psi+H(x,t)\psi, \tag{1}$$

$$H(x,t)=-qE[x(\theta(x)-\theta(x-a))+a\theta(x-a)](e^{i\omega t}+e^{-i\omega t})+q\varphi[x,\psi],$$

where q and m^* are the electron charge and mass, $\alpha=\varphi_b b$, φ_b and b are the height and width of the barrier, $\theta(x)$ is the unit step function, $q\varphi[x,\psi]$ is the change in the potential energy due to the space charge, and $\varphi[x,\psi]$ is a solution of the Poisson equation

$$\frac{\partial^2\varphi[x,\varphi]}{\partial x^2}=-\frac{q}{\varepsilon}\Delta n[\psi], \tag{2}$$

where $\Delta n[\psi]$ is the electron density perturbation in the structure, and ε is the semiconductor dielectric constant. Since the amplitude of the harmonic field is small, all variable parameters should be also harmonic functions of time. In the small-signal approximation, we seek a solution of Eq. (1) with the perturbation

$$H(x,t)=V_-(x)e^{i\omega t}+V_+(x)e^{-i\omega t}$$

in the form[6]

$$\psi=\psi_0+\psi_1=\psi_0(x)e^{-i\omega_0 t}+\psi_+(x)e^{-i(\omega_0+\omega)t}+\psi_-(x)e^{-i(\omega_0-\omega)t},$$

where ψ_0 is the solution for the unperturbed system ($\omega_0=\mathscr{E}/\hbar$, $\mathscr{E}$ is the energy of electrons incident on the structure), and $|\psi_1|\ll|\psi_0|$. Since the perturbation problem is linear, $\psi_1=\psi_1[E]+\psi_1[\varphi]$.

In first-order perturbation theory, the variation in the electron density has the form

$$\Delta n(x,t)=[\psi_0\psi_+^*+\psi_0^*\psi_-]e^{i\omega t}+[\psi_0^*\psi_++\psi_0\psi_-^*]e^{-i\omega t}=2\Delta n(x)\cos[\omega t+\beta(x)]. \tag{3}$$

The functions $\psi_\pm$ in this structure can be expressed as follows:

$$\psi_\pm(x)=\begin{cases}D_\pm\exp[-ik_\pm x], & x<0,\\ A_\pm\sin(k_\pm x)+B_\pm\cos(k_\pm x)+\chi_\pm(x), & 0<x<a,\\ C_\pm\exp[ik_\pm(x-a)]+P_\pm\exp[ik(x-a)], & x>a,\end{cases} \tag{4}$$

where

$$k=\sqrt{\frac{2m^*\mathscr{E}}{\hbar^2}},\quad k_\pm=\sqrt{\frac{2m^*(\omega_0\pm\omega)}{\hbar}},$$

$$P_\pm=\pm\frac{V(a)}{\hbar\omega}\psi_0(a),$$

and $\chi_\pm(x)$ are the particular solutions of the equation[6]

$$\hbar(\omega_0\pm\omega)\psi_\pm(x)=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi_\pm}{\partial x^2}+V_\pm(x)\psi_0(x). \tag{5}$$

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The coefficients $A_\pm$, $B_\pm$, $C_\pm$, and $D_\pm$ are derived by matching the wave function and its derivatives at the barriers at each moment of time.[4,5]

We assume that the perturbation $V_\pm(x)=-qEx/2$ generates a change in the electron density $n_E\xi(x)\cos(\omega t+\beta_1)$, leading to some change in the potential, which in turn modulates the electron flux.

Suppose that the variation in electron density due to the field of the space charge has the same spatial dependence $\xi(x)$ as the variation in density due to the uniform electric field (this assumption can be checked for each specific case by direct calculation). Denoting by $n_q\xi(x)\cos(\omega t+\gamma)$ the density variation related only to the space charge, a uniform, harmonically varying field $E\cos(\omega t)$ will yield a potential energy of the form

$$H(x,t)=-qEx\cos\omega t+\frac{q\varphi_N(x)}{N}[n_E\cos(\omega t+\beta_1)+n_q\cos(\omega t+\gamma)], \tag{6}$$

where

$$\varphi_N(x)=-\frac{qN}{\varepsilon}\int_0^x\int_0^{x'}\xi(x'')dx'dx''+G_1x+G_2.$$

Here N is a normalization factor with dimensions of electron density, and the constants G_1 and G_2 can be derived from the boundary conditions for each specific case.

Let the perturbation $H(x,t)=q\varphi_N(x)\cos(\omega t)$ [$V_\pm=q\varphi_N(x)/2$] correspond to the varying electron density $n_\varphi\xi(x)\cos(\omega t+\beta_2)$. Then the perturbation of the potential energy given by Eq. (6) corresponds to the varying electron density

$$\tilde{n}(t)=n_E\xi(x)\cos(\omega t+\beta_1)+\frac{n_En_\varphi}{N}\xi(x)\cos(\omega t+\beta_1+\beta_2)+\frac{n_qn_\varphi}{N}\xi(x)\cos(\omega t+\beta_2+\gamma). \tag{7}$$

In order to obtain a self-consistent solution, we equate the right-hand side of Eq. (7) and the space charge density, i.e.,

$$\tilde{n}(t)=n(t)=n_q\xi(x)\cos(\omega t+\gamma)+n_E\xi(x)\cos(\omega t+\beta_1), \tag{8}$$

whereupon

$$n_q\cos(\omega t+\gamma)=\frac{n_qn_\varphi}{N}\cos(\omega t+\beta_2+\gamma)+\frac{n_En_\varphi}{N}\times\cos(\omega t+\beta_1+\beta_2). \tag{9}$$

Since this equality hold at each moment of time, the coefficients of both $\cos(\omega t)$ and $\sin(\omega t)$ must be equal, thereby yielding n_q and γ. Thus, the perturbation $V(t)$ in Eq. (6) corresponds to the electron density $n(t)$ given by Eq. (8) and the electron wave functions $\psi=\psi_0+\psi_1(E)+\psi_1(\varphi(n(t)))$.

Following this scheme for the resonant interaction between an electron and ac field in a double-barrier structure, we calculate n_E, $\xi(x)$, and β_1, and verify that the dynamic space charge outside the structure is small.

The equations for the coefficients $A_\pm$, $B_\pm$, $C_\pm$, and $D_\pm$ of the wave functions defined by Eq. (3) can be written in the matrix form as

$$\begin{pmatrix}1 & 0 & -1 & 0\\ ik_\pm-y & k_\pm & 0 & 0\\ 0 & \sin k_\pm a & \cos k_\pm a & -1\\ 0 & -k_\pm\cos k_\pm a & k_\pm\sin k_\pm a & ik_\pm-y\end{pmatrix}\begin{pmatrix}D_\pm\\A_\pm\\B_\pm\\C_\pm\end{pmatrix}=\begin{pmatrix}f_1\\f_2\\f_3\\f_4\end{pmatrix}=\begin{pmatrix}\chi_\pm(0)\\-\chi'_\pm(0)\\P_\pm-\chi_\pm(a)\\(y-ik)P_\pm+\chi'_\pm(a)\end{pmatrix}, \tag{10}$$

where $y=2m^*\alpha/\hbar^2$.

In double-barrier structures the transmission factor has clear-cut resonances, and in symmetric structures it equals unity at values of k that are roots of the transcendental equation[7]

$$\tan ka=-\frac{k\hbar^2}{\alpha m^*}=-\frac{2k}{y}. \tag{11}$$

The unperturbed electron wave function normalized by the electron density n is expressed as

$$\psi_0(x)=\sqrt{n}\begin{cases}\exp[ikx], & x<0,\\ A_0\sin kx+B_0\cos kx, & 0<x<a,\\ C_0\exp[ik(x-a)], & x>a,\end{cases} \tag{12}$$

where

$$A_0=\frac{y}{k}+i,\quad B_0=1,\quad C_0=\left(\frac{y}{k}+i\right)\sin ka+\cos ka.$$

The determinant of the system (10) is

$$\Delta=(2k_\pm^2-y^2)\sin k_\pm a-2k_\pm y\cos k_\pm a+2ik_\pm[k_\pm\cos k_\pm a+y\sin k_\pm a]. \tag{13}$$

Let the electron energy in a monoenergetic flux of electrons pass through a resonant level numbered K, and let the electric field frequency correspond to a transition to level L. If the final state of the transition is a nonresonant level, then $\Delta\sim k_\pm y$, and if the barrier is sufficiently high ($y\ll k_\pm$) and the resonant transition is strong enough, the determinant will be small:

$$\Delta\approx 2ik_\pm^2(-1)^{L+1}.$$

Therefore, narrow resonant levels, only the transition probability between two resonant levels is important. In the case of broad levels ($y\sim k$), transition probabilities with both emission and absorption of a photon of energy $\hbar\omega$ may be comparable.

For $V_\pm(x)=-qEx$ (see Ref. 5),

$$\chi_\pm=\mp\frac{qEx}{\hbar\omega}\psi_0+\frac{qE}{m^*\omega^2}\psi'_0, \tag{14}$$

so with ($y \gg k_\pm$) for resonant transitions, having calculated the function f in Eq. (10) and only retained terms with the highest power in y in (10) and (13), we obtain:

$$D_\pm \approx \frac{qE}{2ik_\pm m^* \omega^2}(ik+y)(ik_\pm - y)[\cos k_\pm a - \cos ka]\sqrt{n}(-1)^{L+1}, \tag{15}$$

$$C_\pm \approx \frac{qE}{2ik_\pm m^* \omega^2}(ik+y)(ik_\pm - y)[\cos k_\pm a \cos ka - 1]\sqrt{n}(-1)^{L+1}. \tag{16}$$

It follows from Eq. (10) that the sign of cos ka changes with level number, so only transitions in which the difference between level numbers is odd are important for a double-barrier resonant tunneling structure with sufficiently high barriers ($y \gg k_\pm$).

It also follows from Eqs. (15) and (16) that the validity criterion for perturbation theory in this problem has the form

$$qEy^2/m^*\omega^2 k_\pm \ll 1$$

or

$$qEa \ll \pi\hbar\omega |K^2 - L^2| k_\pm^2/2y^2 L,$$

i.e., perturbation theory is valid when the classical interaction energy between an electron and hf electric field over the structure length is much less than the difference between resonant levels, and the higher and wider the barriers (therefore, the more narrow the resonant levels), the smaller the field amplitude.

The active conductivity σ of a quantum structure (which is determined by the relationship between the photon emission and absorption probabilities) and the current density $j(a)$ leaving the structure, with the electron wave functions given by Eq. (4), are[5,6]

$$\sigma = \frac{\hbar^2\omega}{2aE^2 m^*}[k_+(|C_+|^2 + |D_+|^2) - k_-(|C_-|^2 + |D_-|^2)], \tag{17}$$

$$j = \frac{q\hbar}{2m^*}\{2kn|C_0|^2 + \sqrt{n}[(k+k_+)C_0 C_+^* + (k+k_-)C_0^* C_-]e^{i\omega t} + \text{c.c.}\}. \tag{18}$$

It follows from a comparison of Eqs. (17) and (18), taking due account of Eqs. (15) and (16), that the induced current in a double-barrier structure, with resonant transitions between narrow levels being responsible for the active conductance, is much higher than the current through the structure boundaries ($\sigma \sim y^4$, $j \sim y^2$). Therefore, as we suggested above, the space charge outside the double-barrier structure has a little effect on the resonant interaction between electrons and hf field.

From Eqs. (15)–(17) the following expression can be derived (ignoring space charge) for the active conductivity of a symmetric double-barrier structure in the case of electron transitions between two resonant levels ($ak_\pm \approx \pi L$):

$$\sigma_{E\pm} \approx \pm \frac{8q^2 m^* \alpha^4 n}{\pi L \hbar^6 \omega^3}[1 - (-1)^{K-L}]. \tag{19}$$

Since only transitions between two levels are important in the case of narrow resonant levels, we consider for simplicity of calculations only transitions between the ground and lowest-lying levels (the final equations will naturally also hold for resonant transitions from the ground state to higher levels). In this case we have the following expressions for the coefficients of the wave function (4):

$$B_-(E) \approx D_-(E) \approx (-1)^{L+1} C_-(E) \approx \frac{qEy^2}{im^*\omega^2 k_-}\sqrt{n}, \tag{20}$$

$$A_-(E) \approx \frac{qEy^3}{im^*\omega^2 k_-^2}\sqrt{n}. \tag{21}$$

Substituting Eqs. (20) and (21) into Eq. (4), taking Eq. (12) into account, and retaining only the lowest-order terms in y, we have from Eq. (3)

$$\Delta n(E) \approx \frac{qEy^4 n}{m^*\omega^2 k_-^2 k} 2 \sin \omega t \sin kx \sin k_- x. \tag{22}$$

According to this equation, the perturbation of the electron density changes sign over the structure length and, since $q<0$, it lags the field variations by a phase shift of $3\pi/2$ ($\beta_1 = -3\pi/2$) and the potential by $\pi/2$.

Now to solve of Eq. (9) in terms of $\Delta n(E)$, we have to calculate the density perturbation $\Delta n(\Delta n(E))$ and verify that it has the same spatial dependence as $\Delta n(E)$.

For a density variation of the form $N \sin kx \sin k_- x$, and noting that the field due to the space charge is weak at the boundary, the potential takes the form

$$\varphi(x) = \frac{qN}{\varepsilon}\left\{\frac{\cos(k-k_-)x}{2(k-k_-)^2} - \frac{\cos(k+k_-)x}{2(k+k_-)^2} - \frac{2kk_-}{(k-k_-)^2(k+k_-)^2}\right\}. \tag{23}$$

If we express $\psi_0 \cos(k-k_-)x$ and $\psi_0 \cos(k+k_-)x$ as sums of sines and cosines, we have terms with the wave vector k_-, which is an eigenvalue of Eq. (5) for this structure.[8] Since in a double-barrier structure with thin, high barriers ($k \ll y$) and a resonant transition between the K- and L-levels (we take for definiteness $K>L$) we have $k \approx Kk_1$, $k_- \approx Lk_1$, $\omega \approx (K^2 - L^2)\omega_1$, and $\omega_1 = \mathscr{E}_1/\hbar$ (where $\mathscr{E}_1$ and k_1 are the height of the first resonant level and the anplitude of the respective electron wave vector), the perturbation $V_-(x) = q\varphi(x)$ can be expressed as

$$V_-(x) \approx V\left\{\frac{\cos(K-L)k_1 x}{2(K-L)^2} - \frac{\cos(K+L)k_1 x}{2(K+L)^2} - \frac{2KL}{(K^2-L^2)^2}\right\}. \tag{24}$$

Here we use the notation $V = q^2 N/\varepsilon k_1^2$. Given that k_- is an eigenvalue of Eq. (5) for this structure , we obtain the particular solution of Eq. (5) after substituting Eq. (24) into Eq. (5):

$$\chi_-=-\frac{2KL}{(K^2-L^2)^2}\frac{V}{\hbar\omega}\psi_0$$
$$-\frac{V}{8\hbar\omega_1(K-L)^2KL}\left\{\psi_0 kx\,\sin(K-L)k_1x+\left[x\psi_0'+\frac{L}{K-L}\psi_0\right]\cos(K-L)k_1x\right\}$$
$$-\frac{V}{8\hbar\omega_1(K+L)^2KL}\left\{\psi_0 kx\,\sin(K+L)k_1x+\left[x\psi_0'+\frac{L}{K+L}\psi_0\right]\cos(K+L)k_1x\right\}. \quad (25)$$

Calculating the functions f in Eq. (10) and retaining the highest-order terms in y (only the term with f_3 contributes), we obtain

$$D_-(V)\approx(-1)^{L+1}C_-(V)\approx\frac{1}{2ik_-}\frac{Va(K^2+L^2)}{4\hbar\omega(K^2-L^2)KL}y^2\sqrt{n}, \quad (26)$$

$$A_-(V)\approx\frac{1}{2ik_-^2}\frac{Va(K^2+L^2)}{4\hbar\omega(K^2-L^2)KL}y^3\sqrt{n}. \quad (27)$$

Taking due account of Eqs. (4) and (12), we derive from Eq. (3)

$$\Delta n(V)\approx\frac{Vay^4}{\hbar\omega kk_-^2}\frac{K^2+L^2}{4KL(K^2-L^2)}\sin\omega t\,\sin kx\,\sin k_-x. \quad (28)$$

Hence, it follows that the variation in the electron density due to the space charge potential lags the latter by $\pi/2$ ($\beta_2=-\pi/2$) and, as was assumed above, it has the same shape as the variation in the electron density due to the uniform electric field. The coefficients n_E and n_φ in Eq. (9) are

$$n_E=-\frac{qEy^4n}{m^*\omega^2k_-^2k},\quad n_\varphi=\frac{q^2N}{\varepsilon k_1^2}\frac{ay^4n}{\hbar\omega k_-^2k}\frac{K^2+L^2}{8KL(K^2-L^2)}. \quad (29)$$

Substituting Eq. (29) into Eq. (9) and noting that $\beta_1=-3\pi/2$ and $\beta_2=-\pi/2$, we obtain

$$\tan\gamma=-\frac{n_\varphi}{N},\quad n_q=\frac{n_En_\varphi}{N}\cos\gamma. \quad (30)$$

For subsequent calculations, it is convenient to introduce the complex charge and potential:

$$n(t)=(N_x+iN_y)e^{i\omega t}+\text{c.c.}, \quad (31)$$

$$\varphi(a,t)=[\varphi_x(a)+i\varphi_y(a)]e^{i\omega t}+\text{c.c.} \quad (32)$$

Then

$$N_x=n_q\cos\gamma, \quad (33)$$

$$N_y=n_E+n_q\sin\gamma, \quad (34)$$

$$\varphi(a)=\varphi(E)+\varphi(N_x)+i\varphi(N_y). \quad (35)$$

Given $\varphi(N)$ in (23) and Eq. (24), we have

$$\varphi_x=-aE-\frac{q}{\varepsilon k_1^2}\frac{4KL}{(K^2-L^2)^2}N_x, \quad (36)$$

$$\varphi_y=-\frac{q}{\varepsilon k_1^2}\frac{4KL}{(K^2-L^2)^2}N_y. \quad (37)$$

As in Eq. (37), the expression for D_- in Eq. (4) can be written

$$D_-=D_-(E)+D_-(V(N_x))+iD_-(V(N_y)). \quad (38)$$

Then substituting Eqs. (20) and (26) into (38), taking into account Eqs. (33), (34), and (29), and writing

$$\zeta=\frac{|\sigma_E|}{\omega\varepsilon},\quad \eta_{KL}=\frac{\pi^2(K^2+L^2)(K^2-L^2)^2}{64K^2L^2}, \quad (39)$$

we obtain

$$D_-=D_-(E)\left\{\frac{1}{1+\eta_{KL}^2\zeta^2}-i\frac{\eta_{KL}\zeta}{1+\eta_{KL}^2\zeta^2}\right\}, \quad (40)$$

$$\varphi(a)=-aE\left\{\frac{1+(\eta_{KL}^2-\eta_{KL})\zeta^2}{1+\eta_{KL}^2\zeta^2}-i\frac{\zeta}{1+\eta_{KL}^2\zeta^2}\right\}. \quad (41)$$

Thus, the variation of the potential (32)

$$\varphi(a,t)=\varphi(a)e^{i\omega t}+\text{c.c.}$$

corresponds to the perturbed part of of the wave function (4) with coefficients

$$B_-\approx D_-\approx(-1)^{L+1}C_-,\quad A_-\approx yD_-/k_-.$$

Given these expressions, one can easily reconstruct the electron wave function under any harmonic potential applied to the structure, such as $U(t)=U\cos\omega t$. In most cases the effect of dynamic space charge on the ac conductivity of the structure (or probability of electron transitions between levels), rather than the electron wave function, is what is desired. The conductivity can be derived directly from Eq. (17), using Eqs. (40) and (41). Generally speaking, this calculation should not use the active specific conductivity σ defined in terms of the hf field amplitude, $\sigma=2W/aE^2$, but the active conductance $G=2W/U^2$, defined in terms of the hf voltage U applied to the structure (here W is the hf power absorbed or emitted by electrons), although again in this case, one can also formally introduce the mean field $E=U/a$ and $\sigma=aG$. Given that $|C_-|=|D_-|$, we therefore find from Eqs. (17), (40), and (41) that

$$G=\frac{\sigma_E}{a}\frac{1+\eta_{KL}^2\zeta^2}{1+(1+2\eta_{KL}^2-2\eta_{KL})\zeta^2+\eta_{KL}^2(1-\eta_{KL})^2\zeta^4} \quad (42)$$

or

$$G=-\frac{\omega\varepsilon}{a}\frac{\zeta+\eta_{KL}^2\zeta^3}{1+(1+2\eta_{KL}^2-2\eta_{KL})\zeta^2+\eta_{KL}^2(1-\eta_{KL})^2\zeta^4}$$
$$=-\frac{\omega\varepsilon}{a}F_{KL}(\zeta). \quad (43)$$

Clearly, regardless of the structure parameters, the effect of the dynamic space charge on the resonant interaction between electrons and an hf electric field in symmetric double-

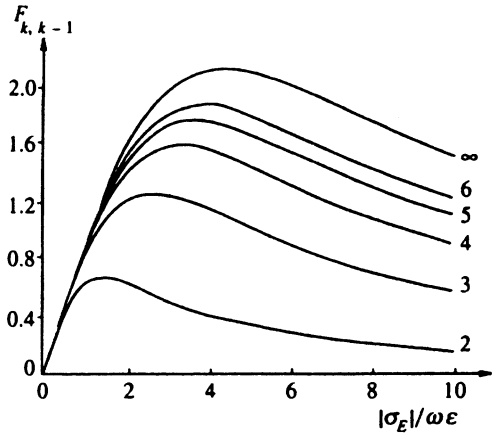

FIG. 1. The function $F_{K,K-1}(|\sigma_E|/\omega\varepsilon)$. The digits indicate numbers of initial resonant levels of transitions.

barrier structures is determined only by the labels of the levels taking part in the transitions and the ratio of the structure conductivity σ_E (19), calculated without the contribution of the space charge, to $\omega\varepsilon$. Plots of $F_{K,K-1}(\zeta)$ are given in Fig. 1. It is clear that in resonant transitions, the peak active conductivity of a double-barrier structure is higher, the higher the levels participating in the transitions. The growth rate of this maximum with the level number is lower at higher levels. For example, $(F_{32})_{\max}/(F_{21})_{\max}\approx 2$, and as $K\to\infty$ the maximum possible conductance is $|G_{\max}|\approx 2.14\omega\varepsilon/a$ (the corresponding conductivity is $|\sigma_E|\approx 4.3\omega\varepsilon$). At $\zeta<0.7\zeta_{\max}$ the space charge has little effect on the transition rate between levels (here $\zeta_{\max}$ is the argument at which the function $F_{K,K-1}(\zeta)$ peaks). At higher $|\sigma_E|/\omega\varepsilon$, the space charge first limits the transition probability and then leads to its decrease.

An analysis of Eq. (43) demonstrates that the dynamic space charge severely limits the transition probability between levels whose labels differ by more than unity. For example, as $K\to\infty$ the maximum of the function $F_{K,K-1}$ is more than 40 times the maximum of $F_{K,K-3}$.

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