Exciton spectrum of surface-corrugated quantum wells: the adiabatic self-consistent approach

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A theory for calculating the relaxation frequency ν and the shift $\delta\omega$ of exciton resonances in quantum wells with finite potential barriers and adiabatic surface disorder is developed. The adiabaticity implies that the correlation length R_c for the well width fluctuations is much larger than the exciton radius a_0 ($R_c \gg a_0$). Our theory is based on the self-consistent Green's function method, and therefore takes into account the inherent action of the exciton scattering on itself. The self-consistent approach is shown to describe quantitatively the sharp exciton resonance. It also gives the qualitatively correct resonance picture for the transition to the classical limit, as well as within the domain of the classical limit itself. We present and analyze results for hh-exciton in a GaAs quantum well with $Al_{0.3}Ga_{0.7}As$ barriers. It is established that the self-consistency and finite height of potential barriers significantly influence on the line-shape of exciton resonances, and make the values of ν and $\delta\omega$ be quite realistic. In particular, the relaxation frequency ν for the ground-state resonance has a *broad*, almost *symmetric* maximum near the resonance frequency ω_0, while the surface-induced resonance shift $\delta\omega$ vanishes near ω_0, and has different signs on the sides of the exciton resonance.

Keywords: Excitons; quantum wells.

Se desarrolla una teoría para calcular la frecuencia de relajación ν y el corrimiento $\delta\omega$ de las resonancias excitónicas en pozos cuánticos con barreras de potencial finitas y desorden superficial adiabático. La adiabaticidad significa que la longitud de correlación R_c para las fluctuaciones del ancho del pozo es mucho mayor que el radio excitónico a_0 ($R_c \gg a_0$). Nuestra teoría se basa en el método de la función autoconsistente de Green y, por lo tanto, toma en cuenta la acción inherente de la dispersión del excitón sobre sí misma. Se muestra que la aproximación autoconsistente describe cuantitativamente la resonancia excitónica aguda. Además, da una descripción cualitativamente correcta de la resonancia durante la transición al límite clásico, así como dentro del dominio del límite clásico mismo. Presentamos y analizamos resultados para el excitón hh en un pozo cuántico de GaAs con barreras de $Al_{0.3}Ga_{0.7}As$. Se establece que la autoconsistencia y la altura finita de las barreras de potencial influyen significativamente sobre la forma de línea de las resonancias excitónicas y hacen que los valores de ν y $\delta\omega$ sean bastante realistas. En particular, la frecuencia de relajación ν para la resonancia del estado base tiene un máximo *ancho*, casi *simétrico* cerca de la frecuencia de resonancia ω_0, mientras que el corrimiento $\delta\omega$ de la resonancia, inducido por la superficie, se anula cerca de ω_0 y tiene signos diferentes a los lados de la resonancia excitónica.

Descriptores: Excitones; pozos cuánticos.

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1. Introduction

In the past few years, the intricate behavior of excitons in surface-disordered semiconductor confined systems (near-surface potential wells [1, 2], thin films [3–6], quantum-well [7–27] and quantum-wire [28] structures) has been intensively investigated. In the regime of weak confinement, the characteristic size d of the system is much larger than the exciton Bohr radius a_0 ($d \gg a_0$). Here, the relative motion of the electron-hole pair is as in the bulk, except for a distortion near sample boundaries at distances of the order of a_0. In this regime, the quantization of the exciton center-of-mass motion occurs giving rise to an specific resonance structure in optical spectra [5, 29–31] (absorption, transmission, specular and diffuse reflection). Surface roughness alters the spectrum of quantized excitons by increasing the damping factor [6,30] and shifting the eigenfrequencies [6]. Consequently, the line-shape and position of exciton resonances in optical spectra are also modified. In the majority of the investigations, it has been assumed that the sample surfaces are adiabatically disordered, *i.e.* the roughness correlation length R_c is much larger than the 3D-exciton radius a_0 [32]:

$$a_0 \ll R_c. \tag{1}$$

This assumption has enabled to construct relatively simple, but rather realistic theories for interpreting optical properties of excitons in surface-disordered systems within the regime of weak confinement.

In systems such as quantum wells, having a size (width) d smaller than the exciton radius a_0 ($d \lesssim a_0$), the regime of strong confinement of excitons is realized. Several phenomenological [21,22,25] and microscopic [10–17,19] theories have been developed for describing the interaction of excitons with the inherently rough surfaces of quantum wells. Microscopic theories are based on the use of the Schrödinger

equation for the exciton in-plane center-of-mass motion in a disordered potential. The problem of scattering of exciton center-of-mass by the rough quantum-well surfaces becomes physically more clear, and can be solved analytically within the adiabatic regime (1) [19]. The microscopic solution of the scattering problem for an arbitrary relation between the exciton radius a_0 and the roughness correlation length R_c can be found either numerically [14, 15], or for the ground-state exciton in quasi-2D quantum wells [26, 27].

In the present work, we develop a theory for the exciton-surface scattering in quasi-2D quantum wells, whose average well width d satisfies the inequality

$$\sigma \ll d < a_0, \tag{2}$$

where σ is the r.m.s. roughness height. Due to the right condition in Eq. (2), the Coulomb interaction is suppressed in the direction perpendicular to the well plane. So, in analyzing the exciton surface scattering, we consider the individual interactions of the electron and hole with the rough surface in presence of their in-plane Coulomb coupling. Unlike the majority of previous studies, the inherent action of the exciton scattering on itself is taken into account here. Therefore, in order to manage the exciton-surface scattering problem we have applied and generalized to the case of two-particle motion, the self-consistent Green's function method. This approach turns out to be the most appropriate for our purposes because it deals with the original microscopic excitonic Hamiltonian, and introduces the *exciton-surface scattering frequency* ν, and the *exciton-resonance shift* $\delta\omega$ in a very natural way.

It should be commented here that the self-consistent Green's function method was applied in some previous works [16–18, 26, 27]. In two of them [16, 17], a *short-range* (δ-like) correlation function for interface fluctuations of *infinitely deep* wells was assumed. In such a case ($R_c \to 0$), both the self-consistent approach and the ordinary (not self-consistent) Born approximation predict qualitatively similar line-shapes for exciton resonances. The advantages of the self-consistent method is, however, better exploited with finite values of the correlation length R_c [26, 27]. In another work [18], the *ground-state exciton* linewidth for a surface-corrugated quantum well with *infinite* barriers was calculated by using the Fermi golden rule and the self-consistent Born approximation. It was shown that the self-consistent approach gives more reasonable values of the linewidth as they are compared with the experiment. In Ref. 18, it was also noted that a better (quantitative) agreement with the experimental results can be achieved *only* if the finiteness of the potential barriers is taken into account. Where applicable, the results of Ref. 18 agree with Refs. 26 and 27, as well as with our present research.

The present theory will be qualitatively restricted to the common situation of adiabatically disordered surfaces (1). As will be shown, in the adiabatic regime, the relaxation frequency ν and the resonance shift $\delta\omega$ of any exciton (not only the ground-state one, but also next excited states) in realistic quantum wells, *i.e.* with *finite* potential barriers and *anisotropic* effective masses of the electron and hole, can be calculated by using relatively simple equations, which are easily analyzable and display explicitly the dependencies of ν and $\delta\omega$ upon the parameters of the exciton, interface roughness, and exciton-resonance detuning. From the analysis performed below, one can come to an interesting conclusion: The type of excitonic resonance and its line-shape are mainly determined by the competition between the correlation properties of surface disorder and the finiteness of potential barriers of a quantum well. The increase of the correlation radius leads towards the broad resonance. Otherwise, the less height of potential barriers the sharper and more asymmetric the resonance.

The formulation of the problem and the details of self-consistent Green's function method applied to the electron-hole motion in quasi-2D quantum wells are exhibited in Secs. 2 and 3. A general expression with its brief analysis for the exciton self-energy, whose real and imaginary parts determine respectively the exciton-resonance shift $\delta\omega$, and the exciton-surface scattering frequency ν is given in Sec. 4. Finally, in Sec. 5 we calculate and analyze the frequency dependencies of ν and $\delta\omega$ for a GaAs quantum well with $Al_{0.3}Ga_{0.7}As$ barriers. Here, the predictions of the self-consistent approach and the ordinary Born approximation are compared. The short report preceding this comprehensive paper has been published in Ref. 33.

2. Problem Statement

We consider a quantum well of average width d, being confined within the region

$$\xi(\vec{r}_{e,h}) \le z_{e,h} \le d. \tag{3}$$

Here, coordinates $z_{e,h}$ specify the transverse to the well (*i.e.* along the growth direction of the well), motion of the electron (e), or the hole (h), respectively. The surface roughness is described by a random function $\xi(\vec{r})$ of the in-plane (electron or hole) position vector $\vec{r}$. The function $\xi(\vec{r})$ is assumed to be a statistically homogeneous and isotropic random process with zero average, which is characterized by standard properties [34],

$$\langle \xi(\vec{r}) \rangle = 0, \qquad \langle \xi(\vec{r}) \xi(\vec{r'}) \rangle = \sigma^2 \mathcal{W}(|\vec{r} - \vec{r'}|). \tag{4}$$

The angular brackets stand for statistical averaging over the ensemble of realizations of the rough-surface-profile function $\xi(\vec{r})$. The symbol σ denotes the root-mean-square (r.m.s.) roughness height. The binary coefficient of correlation $\mathcal{W}(|\vec{r}|)$ has the unit amplitude, $\mathcal{W}(0) = 1$, and a typical scale of decrease R_c (the correlation radius), which is of the order of the mean length of surface irregularities. So, our consideration supposes that the relief $z = \xi(\vec{r})$ of the lower boundary is randomly corrugated while the upper interface, $z = d$, is, for simplicity, flat. However, such a system is physically equivalent to a well with both boundaries being rough,

statistically identical, and not intercorrelated [34]. Moreover, our method can be easily generalized to systems with arbitrary statistical properties of both quantum-well interfaces.

Due to the definition (2) of a quantum well, the excitonic Hamiltonian $\hat{\mathcal{H}}_{QW}$ can be suitably written in the following form

$$\hat{\mathcal{H}}_{QW}=E_{gap}-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\vec{R}^2}-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial\vec{\rho}^2}-\frac{e^2}{\varepsilon_0\rho}-\frac{\hbar^2}{2m_{ez}}\frac{\partial^2}{\partial z_e^2}$$
$$-\frac{\hbar^2}{2m_{hz}}\frac{\partial^2}{\partial z_h^2}+U_e(z_e,\vec{r}_e)+U_h(z_h,\vec{r}_h)-i\hbar\nu_0. \quad (5)$$

Here E_{gap} is the energy gap between the conduction and valence bands of semiconductor, m_{ez} (m_{hz}) is the z-axis electron (hole) effective mass. The second term in the Hamiltonian (5) is the operator of kinetic energy of the exciton center-of-mass motion, which is described by the x-y plane total mass $M = m_{e||} + m_{h||}$, and the in-plane radius vector $\vec{R}$. The third term represents the kinetic energy of the relative electron-hole motion, and is specified by the x-y plane reduced mass $\mu = m_{e||}m_{h||}/M$, and the internal in-plane vector $\vec{\rho}$. The relations connecting the introduced in-plane vectors are

$$\vec{r}_{e,h} = \vec{R} \pm \mu\vec{\rho}/m_{e||,h||}, \qquad \vec{\rho} = \vec{r}_e - \vec{r}_h. \quad (6)$$

To a good approximation, the electron-hole Coulomb interaction is described by the two-dimensional Coulomb potential (the fourth term), with ε_0 being the dielectric constant of the excitonic medium. Indeed, as was noted in Ref. 35, the effect of the finite well width d is negligible when $d < a_0$ (2), since the corrections to the exciton eigenenergies are of the order of $(d/a_0)^2 \ll 1$. The fifth and sixth terms are responsible for the individual transverse motion of the electron or the hole, respectively. The quantities $U_e(z_e,\vec{r}_e)$ and $U_h(z_h,\vec{r}_h)$ are the confining potentials of the quantum well for the electron and the hole,

$$U_{e,h}(z_{e,h},\vec{r}_{e,h}) = U_{e,h}$$
$$\times\left[\Theta(\xi(\vec{R}\pm\frac{\mu}{m_{e||,h||}}\vec{\rho})-z_{e,h})+\Theta(z_{e,h}-d)\right]. \quad (7)$$

Here $U_{e,h}$ is the finite height of the potential barrier for the electron (e) and the hole (h), $\Theta(x)$ is the Heaviside unit-step function. In the Hamiltonian (5), we have introduced a homogeneous exciton-bulk damping $\nu_0 > 0$ to take into account its effect on the exciton-surface scattering.

To analyze properly excitonic states in a surface-corrugated quantum well, we shall derive the retarded Green function $\mathcal{G} = \mathcal{G}(\vec{R},\vec{R}';\vec{\rho},\vec{\rho}';z_e,z_e';z_h,z_h')$ of the Hamiltonian (5). This function obeys the equation

$$(\hbar\omega-\hat{\mathcal{H}}_{QW})\mathcal{G}=\delta(\vec{R}-\vec{R}')\delta(\vec{\rho}-\vec{\rho}')\delta(z_e-z_e')\delta(z_h-z_h'), \quad (8)$$

where $\delta(x)$ is the Dirac delta-function. For convenience of the subsequent averaging, the differential Eq. (8) is reduced to the integral Dyson-type equation that relates the perturbed by surface disorder Green function $\mathcal{G}$ to the Green function $\mathcal{G}_0$ for the ideal well with flat interfaces (with $\xi(\vec{r}) = 0$). The explicit form of the required integral equation is

$$\mathcal{G}(\vec{R},\vec{R}';\vec{\rho},\vec{\rho}';z_e,z_e';z_h,z_h') = \mathcal{G}_0(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho}';z_e,z_e';z_h,z_h') + \int_{-\infty}^{\infty} d^2R_1 \int_{-\infty}^{\infty} d^2\rho_1 \int_{-\infty}^{\infty} dz_{e1} \int_{-\infty}^{\infty} dz_{h1}$$
$$\times\,\mathcal{G}_0(\vec{R}-\vec{R}_1;\vec{\rho},\vec{\rho}_1;z_e,z_{e1};z_h,z_{h1})[V_e(\vec{R}_1,\vec{\rho}_1;z_{e1})+V_h(\vec{R}_1,\vec{\rho}_1;z_{h1})]\mathcal{G}(\vec{R}_1,\vec{R}';\vec{\rho}_1,\vec{\rho}';z_{e1},z_e';z_{h1},z_h'). \quad (9)$$

This equation contains the kernels $V_e(\vec{R}_1,\vec{\rho}_1;z_{e1})$ and $V_h(\vec{R}_1,\vec{\rho}_1;z_{h1})$ that have the meaning of the effective electron-surface and hole-surface scattering potentials, respectively, and take into account the individual interactions of the electron and the hole with the rough interface. Evidently, these scattering potentials are given by the difference between the confining potentials of the corrugated $z = \xi(\vec{r})$, and ideally flat $z = 0$ interfaces

$$V_{e,h}(\vec{R},\vec{\rho};z_{e,h}) = U_{e,h}\left[\Theta(\xi(\vec{R}\pm\frac{\mu}{m_{e||,h||}}\vec{\rho})-z_{e,h})-\Theta(-z_{e,h})\right] = U_{e,h}\,\delta(z_{e,h})\,\xi(\vec{R}\pm\frac{\mu}{m_{e||,h||}}\vec{\rho}). \quad (10)$$

The delta-function $\delta(z_{e,h})$ emerges in Eq. (10) due to the condition $\sigma \ll d$, and shows clearly the surface nature of the scattering potentials $V_{e,h}$.

One of the central points of our approach is that within the adiabatic regime (1) the correlators of the electron-surface V_e and hole-surface V_h scattering operators, having the variation scale R_c, slowly vary over the scale $\rho_0 = \hbar^2\varepsilon_0/2e^2\mu$ ($\sim a_0/2$) of the rapid relative electron-hole motion in the 2D Coulomb potential. Therefore, we can neglect their dependence on the internal vector $\vec{\rho}$. Indeed, in accordance with the definition (10), and the correlation properties (4), these correlators contain the dependence on $\vec{\rho}$ only in the argument of the correlation function $\mathcal{W}$. Since the variation scale $\rho_0 \sim a_0/2$ is much less than the correlation radius R_c, we can put $\vec{\rho} = 0$ everywhere in the argument of $\mathcal{W}$. Therefore, in the adiabatic approximation (1) we

get

$$\langle V_{e,h}(\vec{R},\vec{\rho};z_{e,h})V_{e,h}(\vec{R}',\vec{\rho}';z'_{e,h})\rangle = \sigma^2 U_{e,h}^2\,\delta(z_{e,h})\delta(z'_{e,h})\mathcal{W}(|\vec{R}-\vec{R}'|); \tag{11}$$

$$\langle V_{e,h}(\vec{R},\vec{\rho};z_{e,h})V_{h,e}(\vec{R}',\vec{\rho}';z'_{h,e})\rangle = \sigma^2 U_e U_h\,\delta(z_{e,h})\delta(z'_{h,e})\mathcal{W}(|\vec{R}-\vec{R}'|). \tag{12}$$

As follows from the statistical homogeneity and isotropy of the scattering potentials V_e and V_h with respect to the exciton center-of-mass position vector $\vec{R}$ [see Eqs. (11) and (12)], the average Green function $\langle\mathcal{G}(\vec{R},\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h)\rangle$ also turns out to be uniform and isotropic in the exciton center-of-mass radius vector $\vec{R}$:

$$\langle\mathcal{G}(\vec{R},\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h)\rangle = \overline{\mathcal{G}}(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h). \tag{13}$$

To derive the equation for $\overline{\mathcal{G}}$ we average the exact Eq. (9) for G. To this end one can use methods developed in the spectral theory of surface-disordered systems, such as the perturbative diagrammatic method (see, *e.g.*, Refs. 34 and 36), or the technique proposed in Ref. 37. Both of the methods allow to take adequately into account the effects of *multiple scattering* of electron and hole from the corrugated surface. As a result, the integral equation for the averaged Green function within the self-consistent Born approximation in the perturbation operator $V_e + V_h$ can be explicitly written as

$$\overline{\mathcal{G}}(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h) = \mathcal{G}_0(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h) + \int_{-\infty}^{\infty} d^2R_1 \int_{-\infty}^{\infty} d^2R_2 \int_{-\infty}^{\infty} d^2\rho_1 \int_{-\infty}^{\infty} d^2\rho_2 \int_{-\infty}^{\infty} dz_{e1}$$
$$\times \int_{-\infty}^{\infty} dz_{e2} \int_{-\infty}^{\infty} dz_{h1} \int_{-\infty}^{\infty} dz_{h2}\mathcal{G}_0(\vec{R}-\vec{R}_1;\vec{\rho},\vec{\rho}_1;z_e,z_{e1};z_h,z_{h1})\mathcal{M}(\vec{R}_1-\vec{R}_2;\vec{\rho}_1,\vec{\rho}_2;z_{e1},z_{e2};z_{h1},z_{h2})$$
$$\times\overline{\mathcal{G}}(\vec{R}_2-\vec{R}';\vec{\rho}_2,\vec{\rho}';z_{e2},z'_e;z_{h2},z'_h). \tag{14}$$

Here, the self-energy kernel $\mathcal{M}$ has the form

$$\mathcal{M}(\vec{R}_1-\vec{R}_2;\vec{\rho}_1,\vec{\rho}_2;z_{e1},z_{e2};z_{h1},z_{h2}) = \langle(\hat{V}_e+\hat{V}_h)\overline{\mathcal{G}}(\hat{V}_e+\hat{V}_h)\rangle = \sigma^2\,\mathcal{W}(|\vec{R}_1-\vec{R}_2|)\,[U_e\delta(z_{e1})+U_h\delta(z_{h1})]$$
$$\times\overline{\mathcal{G}}(\vec{R}_1-\vec{R}_2;\vec{\rho}_1,\vec{\rho}_2;z_{e1},z_{e2};z_{h1},z_{h2})\,[U_e\delta(z_{e2})+U_h\delta(z_{h2})]\,. \tag{15}$$

Note that within the ordinary Born approximation the self-energy contains the unperturbed Green function $\mathcal{G}_0$, while in the self-consistent approach $\mathcal{G}_0$ is replaced by $\overline{\mathcal{G}}$.

3. Average Green Function

One can see that the self-energy $\mathcal{M}$ depends only on the difference $\vec{R}_1-\vec{R}_2$ between the exciton center-of-mass position vectors, and its dependence on the internal exciton vectors $\vec{\rho}_1$ and $\vec{\rho}_2$, due to the adiabaticity, is contained only in $\overline{\mathcal{G}}$. This fact allows to seek the average Green function $\overline{\mathcal{G}}$ in the form of a Fourier integral over the in-plane exciton center-of-mass wave vector $\vec{k_t}$, and a series over the 2D Coulomb modes,

$$\overline{\mathcal{G}}(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho}';z_e,z'_e;z_h,z'_h) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\Phi_{nm}(\vec{\rho})\,\Phi^*_{nm}(\vec{\rho}')\int_{-\infty}^{\infty}\frac{d^2k_t}{(2\pi)^2}\,\exp[i\vec{k_t}(\vec{R}-\vec{R}')]\,\overline{G}(\vec{k_t};n;z_e,z'_e;z_h,z'_h). \tag{16}$$

Here, $\Phi_{nm}(\vec{\rho})$ are the eigenfunctions (2D Coulomb modes) for the exciton intrinsic motion in the 2D Coulomb potential, with n and m being radial (energy), and azimuth quantum numbers, respectively. The asterisk "$*$" stands for the complex conjugation. Evidently, the unperturbed Green function $\mathcal{G}_0$ can be expressed in the same way as Eq. (16) representation, but with $G_0(\vec{k_t};n;z_e,z'_e;z_h,z'_h)$ instead of $\overline{G}(\vec{k_t};n;z_e,z'_e;z_h,z'_h)$.

According to Eq. (14) the average Green function $\overline{G}$ is governed by the equation

$$\overline{G}(\vec{k_t};n;z_e,z'_e;z_h,z'_h) = G_0(\vec{k_t};n;z_e,z'_e;z_h,z'_h) + \int_{-\infty}^{\infty} dz_{e1} \int_{-\infty}^{\infty} dz_{e2} \int_{-\infty}^{\infty} dz_{h1} \int_{-\infty}^{\infty} dz_{h2}\,G_0(\vec{k_t};n;z_e,z_{e1};z_h,z_{h1})$$
$$\times\mathcal{M}(\vec{k_t};n;z_{e1},z_{e2};z_{h1},z_{h2})\,\overline{G}(\vec{k_t};n;z_{e2},z'_e;z_{h2},z'_h). \tag{17}$$

The self-energy $\mathcal{M}$ in the $\{\vec{k}_t, n, m\}$-representation is given by

$$\mathcal{M}(\vec{k}_t; n; z_{e1}, z_{e2}; z_{h1}, z_{h2}) = [U_e\delta(z_{e1}) + U_h\delta(z_{h1})]\,[U_e\delta(z_{e2}) + U_h\delta(z_{h2})]\,\sigma^2 \times \int_{-\infty}^{\infty} \frac{d^2k'_t}{(2\pi)^2}\, W(|\vec{k}_t - \vec{k}'_t|)\,\overline{G}(\vec{k}'_t; n; z_{e1}, z_{e2}; z_{h1}, z_{h2}). \quad (18)$$

In this expression, we have introduced the Fourier transform $W(|\vec{k}_t|)$ of the binary coefficient of correlation $\mathcal{W}(|\vec{R}|)$,

$$W(|\vec{k}_t|) = \int_{-\infty}^{\infty} d^2R\, \exp(-i\vec{k}_t\vec{R})\,\mathcal{W}(|\vec{R}|) = 2\pi R_c^2 \int_0^{\infty} x dx \mathcal{W}(R_c x)\, J_0(|\vec{k}_t|R_c x), \quad (19)$$

where $J_0(x)$ is the zero-order Bessel function. Note that the function $\mathcal{W}(R_c x)$ is the dimensionless correlation function of the dimensionless variable x with the scale of decrease of the order of unity.

We should note that the average Green function turns out to be a diagonal matrix in the representation of the 2D Coulomb modes, and the self-energy (18) does not contain the transitions between different Coulomb modes as it would take place in a general case. This means that the relative electron-hole quantum state is conserved at the adiabatic (with respect to the 2D Coulomb potential) exciton-surface interaction. This conclusion is in total agreement with the general theory of adiabatic perturbations [38]. Besides, since the unperturbed exciton states are degenerated over the discrete Coulomb azimuth quantum number m, and the adiabatic exciton-surface scattering does not result in the transitions between Coulomb modes, we can seriously expect that the perturbed states should also be degenerated over the azimuth number m. That is why we do not write the variable m in the arguments of the mode Green function $\overline{G}(\vec{k}_t; n; z_e, z'_e; z_h, z'_h)$ and the self-energy $\mathcal{M}(\vec{k}_t; n; z_{e1}, z_{e2}; z_{h1}, z_{h2})$.

In order to solve Eq. (17), we express the perturbed $\overline{G}(\vec{k}_t; n; z_e, z'_e; z_h, z'_h)$ and unperturbed $G_0(\vec{k}_t; n; z_e, z'_e; z_h, z'_h)$ Green functions in the form of a double series in the complete set of orthonormal confinement eigenfunctions $\Psi^{(e)}_{n_e}(z_e)$ and $\Psi^{(h)}_{n_h}(z_h)$ for the individual transverse motion of the electron (e) and the hole (h),

$$\overline{G}(\vec{k}_t; n; z_e, z'_e; z_h, z'_h) = \sum_{n_e, n'_e=1}^{N_e} \Psi^{(e)}_{n_e}(z_e)\Psi^{(e)*}_{n'_e}(z'_e) \times \sum_{n_h, n'_h=1}^{N_h} \Psi^{(h)}_{n_h}(z_h)\Psi^{(h)*}_{n'_h}(z'_h)\overline{g}(\vec{k}_t; n; n_e, n'_e; n_h, n'_h); \quad (20)$$

$$G_0(\vec{k}_t; n; z_e, z'_e; z_h, z'_h) = \sum_{n_e, n'_e=1}^{N_e} \Psi^{(e)}_{n_e}(z_e)\Psi^{(e)*}_{n'_e}(z'_e)\,\delta_{n_e n'_e} \times \sum_{n_h, n'_h=1}^{N_h} \Psi^{(h)}_{n_h}(z_h)\Psi^{(h)*}_{n'_h}(z'_h)\delta_{n_h n'_h} g_0(\vec{k}_t; n; n_e; n_h). \quad (21)$$

Here, we have introduced the Kronecker delta-symbols $\delta_{n_e n'_e}$, $\delta_{n_h n'_h}$ and the unperturbed Green function $g_0(\vec{k}_t; n; n_e; n_h)$ in the eigenstate representation,

$$g_0^{-1}(\vec{k}_t; n; n_e; n_h) = \hbar\left[\omega - \omega_{n_e n_h}(n) - \left(\frac{\hbar k_t^2}{2M}\right) + i\nu_0\right]. \quad (22)$$

The third term in Eq. (22) is the kinetic energy of the infinite motion of the exciton center of mass, and $\hbar\omega_{n_e n_h}(n)$ is the eigenvalue of the total exciton energy $\hbar\omega$,

$$\omega_{n_e n_h}(n) = \frac{E_{gap}}{\hbar} + \frac{E_{2D}(n)}{\hbar} + \frac{\hbar k_{ze}^2(n_e)}{2m_{ez}} + \frac{\hbar k_{zh}^2(n_h)}{2m_{hz}}. \quad (23)$$

The quantity $E_{2D}(n)$ is the eigenenergy of the exciton intrinsic motion originated from the electron-hole Coulomb interaction,

$$E_{2D}(n) = -\frac{e^4\mu}{2\hbar^2\varepsilon_0^2(n+1/2)^2}, \quad (24)$$

which is degenerated over the discrete azimuth quantum number m. The third and fourth terms in Eq. (23) denote the quantized energies of the transverse electron and hole motions, respectively. The integers N_e, N_h are the numbers of levels of the transverse quantization for the electron and hole. Note that the Green coefficient g_0 does not depend on the azimuth quantum number m due to the degeneration of the exciton eigenenergy over it.

After substituting Eqs. (20) and (21) into the adiabatic Dyson equation (17), we get the new one for the Green matrix $\overline{g}(\vec{k}_t; n; n_e, n'_e; n_h, n'_h)$,

$$\overline{g}(\vec{k}_t; n; n_e, n'_e; n_h, n'_h) = g_0(\vec{k}_t; n; n_e; n_h)\delta_{n_e n'_e}\delta_{n_h n'_h} + g_0(\vec{k}_t; n; n_e; n_h) \sum_{n_{e1}=1}^{N_e} \sum_{n_{h1}=1}^{N_h} \mathcal{M}_{n_e n_{e1}; n_h n_{h1}}(\vec{k}_t; n) \times \overline{g}(\vec{k}_t; n; n_{e1}, n'_e; n_{h1}, n'_h), \quad (25)$$

where the self-energy matrix $\mathcal{M}_{n_e n_{e1}; n_h n_{h1}}(\vec{k}_t; n)$ is defined

by

$$\mathcal{M}_{n_e n_{e1};n_h n_{h1}}(\vec{k_t};n) = \sigma^2 \int\limits_{-\infty}^{\infty} \frac{d^2k'_t}{(2\pi)^2} W(|\vec{k_t}-\vec{k'_t}|) \times \sum_{n_{e2},n_{e3}=1}^{N_e} \sum_{n_{h2},n_{h3}=1}^{N_h} X^*_{(n_e n_h)(n_{e2}n_{h2})} \times \overline{g}(\vec{k'_t};n;n_{e2},n_{e3};n_{h2},n_{h3}) X_{(n_{e1}n_{h1})(n_{e3}n_{h3})}. \quad (26)$$

Here, the adiabatic matrix element $X_{(n_e n_h)(n'_e n'_h)}$ of the exciton-surface interaction is written as

$$X_{(n_e n_h)(n'_e n'_h)} = U_e \Psi^{(e)}_{n_e}(0)\Psi^{(e)*}_{n'_e}(0)\,\delta_{n_h n'_h} + U_h \Psi^{(h)}_{n_h}(0)\Psi^{(h)*}_{n'_h}(0)\,\delta_{n_e n'_e}. \quad (27)$$

Note that within the adiabatic regime the matrix elements (27) turn out to be independent of the Coulomb quantum numbers n, m and the in-plane center-of-mass wave vector $\vec{k_t}$.

Assuming the exciton-surface scattering to be weak, one can conclude that in the first-order approximation in the small adiabatic self-energy $\mathcal{M}$ the solution of Eq. (25) is represented by the diagonal matrix

$$\overline{g}(\vec{k_t};n;n_e,n'_e;n_h,n'_h) = \frac{\delta_{n_e n'_e}\delta_{n_h n'_h}}{g_0^{-1}(\vec{k_t};n;n_e;n_h) - \mathcal{M}_{n_e n_h}(\vec{k_t};n)}, \quad (28)$$

where $\mathcal{M}_{n_e n_h}(\vec{k_t};n)$ is the diagonal element of the self-energy matrix (26).

Now, we summarize the calculations performed above. In accordance with the Eqs. (16), (20), (28), and (22) we can write down the adiabatic Green function in the form

$$\overline{\mathcal{G}}(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho'};z_e,z'_e;z_h,z'_h) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \Phi_{nm}(\vec{\rho})\Phi^*_{nm}(\vec{\rho'}) \sum_{n_e=1}^{N_e} \Psi^{(e)}_{n_e}(z_e)\Psi^{(e)*}_{n_e}(z'_e) \sum_{n_h=1}^{N_h} \Psi^{(h)}_{n_h}(z_h)\Psi^{(h)*}_{n_h}(z'_h) \times \int\limits_{-\infty}^{\infty} \frac{d^2k_t}{(2\pi)^2} \frac{\exp[i\vec{k_t}(\vec{R}-\vec{R}')]}{\hbar\left[\omega - \omega_{n_e n_h}(n) - (\hbar k_t^2/2M) + i\nu_0 - \mathcal{M}_{n_e n_h}(\vec{k_t};n)/\hbar\right]}. \quad (29)$$

Within the self-consistent approach, this expression for $\overline{\mathcal{G}}(\vec{R}-\vec{R}';\vec{\rho},\vec{\rho'};z_e,z'_e;z_h,z'_h)$ should be complemented by the equation for the self-energy $\mathcal{M}_{n_e n_h}(\vec{k_t};n)$. Substituting Eqs. (29) and (27) into the definition (26), we obtain

$$\mathcal{M}_{n_e n_h}(\vec{k_t};n)/\hbar = \frac{\sigma^2}{\hbar^2}\left[U_e|\Psi^{(e)}_{n_e}(0)|^2 + U_h|\Psi^{(h)}_{n_h}(0)|^2\right]^2 \int\limits_{-\infty}^{\infty} \frac{d^2k'_t}{(2\pi)^2} \frac{W(|\vec{k_t}-\vec{k'_t}|)}{\omega - \omega_{n_e n_h}(n) - (\hbar k_t'^2/2M) + i\nu_0 - \mathcal{M}_{n_e n_h}(\vec{k'_t};n)/\hbar}. \quad (30)$$

As we expected, the self-energy $\mathcal{M}_{n_e n_h}(\vec{k_t};n)$ turns out to be independent of the azimuth Coulomb quantum number m. Thus, the adiabatic in the Coulomb potential perturbation does not destroy the Coulomb degeneration of the exciton eigenstates. In addition, in Eq. (30) we have dropped the summation over electron and hole quantum numbers n'_e, n'_h. The inequality $d \ll R_c$, which follows from Eqs. (2) and (1) implies that the exciton-surface scattering is adiabatic not only with respect to relative electron-hole Coulomb motion, but also with respect to their individual transverse motion. Then, the main contribution in the sum over n'_e, n'_h is provided by the term with $n'_e = n_e$ and $n'_h = n_h$.

So, the average Green function (29) contains only a single summation over the Coulomb quantum numbers n, m as well as over the transverse quantum numbers n_e, n_h. Now, we can conclude that the reason for canceling the second summation is the adiabaticity of the electron-surface and hole-surface scattering potentials. The adiabaticity clearly manifests itself in the equation for the self-energy (30), where the summation over the adiabatic quantum numbers n, m and n_e, n_h is altogether absent. Indeed, in accordance with the general quantum theory, in the case of adiabatic perturbation the discrete quantum numbers are conserved and only continuous quantum numbers should change due to scattering [38]. In the problem of exciton-surface scattering such a quantum number is the in-plane exciton center-of-mass wave vector $\vec{k_t}$.

4. Complex Shift of Excitonic Spectrum

As follows from the expression (29) for the average Green function, the surface-induced complex correction to the unperturbed excitonic spectrum $\hbar\omega = \hbar\omega_{n_e n_h}(n)$ of a quantum well is determined by the self-energy $\mathcal{M}_{n_e n_h}(\vec{k_t};n)$. Its real part is responsible for the shift $\delta\omega_{n_e n_h}(n)$ of the excitonic resonance frequency while the imaginary part gives the exciton-surface scattering frequency $\nu_{n_e n_h}(n)$,

$$\delta\omega_{n_e n_h}(n) = \frac{\Re\mathcal{M}_{n_e n_h}(n)}{\hbar},$$

$$\nu_{n_e n_h}(n) = -\frac{\Im \mathcal{M}_{n_e n_h}(n)}{\hbar}. \quad (31)$$

Therefore, to analyze these quantities we should solve the integral Eq. (30), which is rather complicated for the analysis. Nevertheless, it can be substantially simplified if the following facts are taken into account. In optical applications the in-plane wave vector $\vec{k_t}$ turns out to be equal to the longitudinal wave vector of light and hence, its value, in general, is of the order of the light wave number. Therefore, we can consider k_t as the smallest wave number of our problem. In particular, we suppose that the following conditions hold

$$k_t R_c \ll 1, \quad \hbar k_t^2/2M \ll \min\{\omega, \omega_{n_e,n_h}(n)\}, \quad \hbar k_t^2/2M \ll \max\{\nu_0, |\mathcal{M}|/\hbar\}. \quad (32)$$

Under these conditions we can put $\vec{k_t} = 0$ in the argument of the correlator W and $\vec{k_t} = \vec{k_t'} = 0$ in the argument of $\mathcal{M}$ in the Eq. (30). Then we rewrite the integral over $\vec{k_t'}$ in polar coordinates $\{k_t', \varphi\}$, take the integral over φ and change the integration variable k_t' with $\omega_t = \hbar k_t'^2/2M$. Afterwards, we obtain a simpler (not integral) equation for the adiabatic self-energy $\mathcal{M}_{n_e n_h}(n)$,

$$\mathcal{M}_{n_e n_h}(n)/\hbar = \nu_N^2 \frac{M}{\hbar} \times \int_0^\infty \frac{d\omega_t}{2\pi} \frac{W(\sqrt{2M\omega_t/\hbar})}{\omega - \omega_{n_e n_h}(n) - \omega_t + i\nu_0 - \mathcal{M}_{n_e n_h}(n)/\hbar}. \quad (33)$$

Here, the Fourier transform $W(\sqrt{2M\omega_t/\hbar})$ as a function of integration variable, ω_t has the maximal value $W(0) \sim R_c^2$ and the scale of decrease ω_W,

$$\omega_W = \hbar R_c^{-2}/2M. \quad (34)$$

In Eq. (33) we have introduced the normalization frequency ν_N by the expression

$$\nu_N = \frac{\sigma}{\hbar}\left[U_e |\Psi_{n_e}^{(e)}(0)|^2 + U_h |\Psi_{n_h}^{(h)}(0)|^2\right]. \quad (35)$$

This frequency controls the effect of finiteness of potential barriers, the effect of transverse electron and hole quantization on the inhomogeneous shift $\delta\omega_{n_e n_h}(n)$, and broadening $\nu_{n_e n_h}(n)$ of excitonic resonances. According to the surface origin of the exciton scattering potentials (10), the characteristic frequency ν_N contains the confinement eigenfunctions $\Psi_{n_{e,h}}^{(e,h)}(0)$ for the electron (e) and the hole (h) taken at the unperturbed well interface $z_{e,h} = 0$. It is noteworthy that for infinitely deep quantum wells when $U_{e,h} = \infty$ and $\Psi_{n_{e,h}}^{(e,h)}(0) = 0$, the product $U_{e,h}|\Psi_{n_{e,h}}^{(e,h)}(0)|^2$ has finite value, $U_{e,h}|\Psi_{n_{e,h}}^{(e,h)}(0)|^2 = (2/d)\hbar^2(\pi n_{e,h}/d)^2/2m_{ez,hz}$. In this way, the results (33), and (35) provide the transition from the finite to the infinite potential barriers.

In what follows, the exciton-surface scattering frequency $\nu_{n_e n_h}(n)$ is assumed to prevail over the homogeneous broadening ν_0 ($\nu_0 \ll \nu_{n_e n_h}(n)$). Evidently, only such a situation is reasonable when studying the effect of rough interfaces on the broadening and shift of excitonic resonances in quantum wells. One can see from Eq. (33) that the line-shape of excitonic resonances in $\delta\omega_{n_e n_h}(n)$ and $\nu_{n_e n_h}(n)$ is determined by the relation between the values of ω_W and ν_N. When the normalization frequency ν_N is less than the scaling frequency ω_W ($\nu_N^2 \ll \omega_W^2$), the excitonic resonance is *sharp* and *asymmetric*. Here, at the resonance point

$$\omega = \omega_{n_e n_h}(n) + \delta\omega_{n_e n_h}(n)$$

the surface scattering frequency $\nu_{n_e n_h}(n)$ has a value of the order of ν_N^2/ω_W, and the resonance shift is negative,

$$\delta\omega_{n_e n_h}(n) \sim -\nu_{n_e n_h}(n) \ln(\omega_W/\nu_{n_e n_h}(n)).$$

As the frequencies ω_W and ν_N approach each other, the excitonic resonance in $\nu_{n_e n_h}(n)$ is enhanced, becoming more symmetric, and the relaxation frequency tends to its maximal value equal to ν_N. At the same time, the resonance shift $\delta\omega_{n_e n_h}(n)$ vanishes.

It should be noted that the self-consistent approximation is rigorously justified if the resonance term in Eq. (33) is a sharper function than the Fourier transform of the binary correlator. From the analysis performed above, this suggests that the condition $\nu_N < \omega_W$ should hold. In the opposite case when $\omega_W \ll \nu_N$, the theory should be constructed within the so-called *classical limit*. As is known from Refs. 14, 39, and 40, in this region the resonance is *broad* and almost *symmetric*. The surface scattering frequency reaches its largest value and the imaginary part of the resonant Green-function coefficient, $\Im\overline{g}(\vec{k_t} = 0; n; n_e; n_h)$, which determines the optical absorptivity, follows the distribution function of surface roughness. We should emphasize that the theory of the classical limit needs further development because the earlier investigations have been restricted just to the consideration of the *exciton ground state* in *infinitely deep* wells with *Gaussian surface disorder*, and the study has been realized by *numeric simulations*. Evidently, this development is a problem of especial research. Here, we would like to draw attention to the fact that our self-consistent Eqs. (29), (33), being applied to the region of broad resonance, give qualitatively correct results. Indeed, when $\omega_W \ll \nu_N$ in the resonance vicinity, the self-energy (33) and the resonant Green-function coefficient $\overline{g}(\vec{k_t} = 0; n; n_e; n_h)$ from Eq. (29) are related by the expression

$$\frac{\mathcal{M}_{n_e n_h}(n)}{\hbar} = \nu_N^2 \overline{g}(\vec{k_t} = 0; n; n_e; n_h) = \frac{\omega - \omega_{n_e n_h}(n)}{2} - i\sqrt{\nu_N^2 - \frac{(\omega - \omega_{n_e n_h}(n))^2}{4}}. \quad (36)$$

So that the imaginary part of the Green-function coefficient turns out to be

$$\Im\overline{g}(\vec{k_t}{=}0; n; n_e; n_h){=}-\nu_N^{-1}\sqrt{1-\frac{(\omega-\omega_{n_e n_h}(n))^2}{4\nu_N^2}}. \quad (37)$$

One can see that the line-shape of the excitonic resonance is symmetric, the real resonance shift is absent and the broadening reaches its maximal value $2\nu_N$. Therefore, the quantity ν_N can be regarded as the exciton-surface scattering frequency for the classical limit. It generalizes the corresponding result obtained in Refs. 14, 39, and 40. The only (but substantial) distinction from the predecessors is that the line-shape is ellipsoidal instead of coinciding with the line-shape of the roughness distribution function. So, if one is interested just in qualitative (rather than exact) description of the excitonic resonance, the self-consistent expressions (29), (33) can be used independently of the ratio between ν_N and ω_W.

The qualitative agreement between the rigorous theory of the classical limit and the corresponding consideration within the self-consistent Born approximation can be naturally explained in the following way. Within the former approach, the results are obtained by the exact summation of all terms in the perturbative expansion for the average Green function [14] reducing this expansion to a convolution of the roughness Gaussian probability density and the unperturbed Green function. Otherwise, the latter approximation sums up accurately only the "dangerous" (of the highest singularity) diagrammatic terms in the series for the self-energy. Evidently, the contribution of these specific terms is the main one, and therefore, provides a qualitatively correct description of the exciton-surface scattering within the classical limit.

After analyzing Eq. (33), we come to a very interesting and non-trivial conclusion: The type of excitonic resonance and its line-shape are determined by the *competition between the adiabaticity of the surface disorder and the finiteness of potential barriers of the quantum well*. The increase of the adiabaticity (the decrease of ω_W) leads towards the broad and symmetric resonance. Otherwise, the less height of potential barriers (the smaller ν_N), the sharper and more asymmetric resonance. That is why the consideration of finite values for the roughness correlation length R_c, and for the height of the potential barriers $U_{e,h}$ is a fundamental requirement to construct an adequate theory of exciton-surface interaction.

It should also be emphasized that the here described features of the excitonic resonances are specific predictions of the *self-consistent approach*, which takes into account the inherent action of exciton-surface scattering on itself. Indeed, within the usual Born approximation, Eq. (33) goes over into a similar one, but with $\mathcal{M}_{n_e n_h}(n) = 0$ in the denominator of the integrand therein. This fact crucially changes the parameter controlling the type of the resonance. Now, it is the ratio between ω_W and the homogeneous bulk broadening ν_0 alone. Evidently, this ratio does not depend on the finiteness of potential barriers. In the next section we show by numerical simulations the principal difference between our self-consistent results and those obtained within usual Born approximation. We also show that for realistic values of the parameters of quantum wells and adiabatic interface roughness, the broad symmetric resonance is more typical than the sharp asymmetric one.

5. Numerical Results and Discussion

Here, in solving Eq. (33) numerically, we shall use a Gaussian correlation function $\mathcal{W}(|\vec{r}|) = \exp(-r^2/R_c^2)$, for which

$$W(|\vec{k_t}|) = \pi R_c^2 \exp(-|\vec{k_t}|^2 R_c^2/4),$$
$$W(\sqrt{2M\omega_t/\hbar}) = \pi R_c^2 \exp(-\omega_t/4\omega_W). \qquad (38)$$

Hence, the Eq. (33) for the self-energy can be rewritten in the form

$$\mathcal{M}_{n_e n_h}(n)/\hbar = \frac{\pi \nu_N^2}{2\omega_W} \int_0^\infty \frac{d\omega_t}{2\pi} \times \frac{\exp(-\omega_t/4\omega_W)}{\omega - \omega_{n_e n_h}(n) - \omega_t + i\nu_0 - \mathcal{M}_{n_e n_h}(n)/\hbar}. \qquad (39)$$

We shall present the calculated frequency dependencies of the broadening $\nu_{n_e n_h}(n)$ and shift $\delta\omega_{n_e n_h}(n)$ of the ground-state hh-exciton resonance ($n_e = 1$, $n_h = 1$, $n = 0$) for a GaAs quantum well of thickness $d = 60$ Å with $Al_xGa_{1-x}As$ ($x = 0.3$) barriers [Curves (a) in Figs. 1–4]. The band gap is calculated by employing the formula $E_{gap}(x) = [1.52 + 1.36x + 0.22x^2]$ eV. The band-gap offset considered in the calculations is 60% for the conduction band and 40% for the valence band. In applying the theory, developed in the preceding sections, we have used identical effective masses for the quantum well and the barriers [41, 42]. So, the effective electron mass $m_{ez} = m_{e||} = 0.067m_0$ (here m_0 is the free electron mass), the x-y plane heavy-hole mass $m_{hh,||} = 0.1m_0$, the z-axis heavy-hole mass $m_{hh,z} = 0.45m_0$. Besides, the rough surface of the quantum well is characterized by a correlation radius $R_c = 500$ Å, much larger than the 2D-exciton radius ρ_0 ($\rho_0 \sim a_0/2$), and a small r.m.s. roughness height $\sigma = 2$ Å. We have also used a homogeneous damping factor $\hbar\nu_0 = 0.1$ meV and $\varepsilon_0 = 12.5$.

As is seen in Fig. 1(curve (a)), the line-shape of the inhomogeneous broadening $\nu \equiv \nu_{1,1}(0)$ for the ground-state exciton resonance is almost *symmetric* with respect to the resonance frequency $\omega_0 \equiv \omega_{1,1}(0) \approx 1.5886$ eV. Besides, the damping ν has a *broad* maximum at a frequency very close to ω_0. As was commented above, such behavior of ν should be observed when the characteristic scaling frequency ω_W (34) of the roughness power spectrum is much smaller than the normalization frequency ν_N (35). It should be emphasized that this condition is well satisfied by the chosen parameters because here $\omega_W \approx \nu_0$ and $\hbar\nu_N \sim 3.6$ meV. Therefore, the maximum of the inhomogeneous broadening ν is well described by the simple formula

$$\nu_{\max} = \frac{\sigma}{\hbar}\left[U_e|\Psi_1^{(e)}(0)|^2 + U_h|\Psi_1^{(h)}(0)|^2\right], \qquad (40)$$

which follows directly from Eqs. (31), (36) and (35). Curve (b) of Fig. 1 exhibits the corresponding inhomogeneous broadening ν as a function of the resonance detuning $\omega - \omega_0$ for the case of ideally infinite barriers (here

$\omega_0 = \omega_{1,1}(0) \approx 1.6886$ eV). In accordance with the analysis performed in the previous section, Fig. 1 shows the exciton-surface scattering frequency ν to be much smaller for finite barriers (curve (a)) than for infinite ones (curve (b)). Therefore, in the latter case the inequality $\omega_W \ll \nu_N$ is better satisfied and the *symmetric* exciton resonance is much broader. Curve (a) of Fig. 2 shows the behavior of the shift $\delta\omega \equiv \delta\omega_{1,1}(0)$ for the GaAs quantum well with $Al_{0.3}Ga_{0.7}As$ barriers. Under the condition of the *broad* resonance $\omega_W \ll \nu_N$, the surface-induced resonance shift $\delta\omega$ vanishes near ω_0, and has different signs on the left and right sides of the excitonic resonance. Consequently, the main effect of $\delta\omega$ on the excitonic resonance turns out to be similar

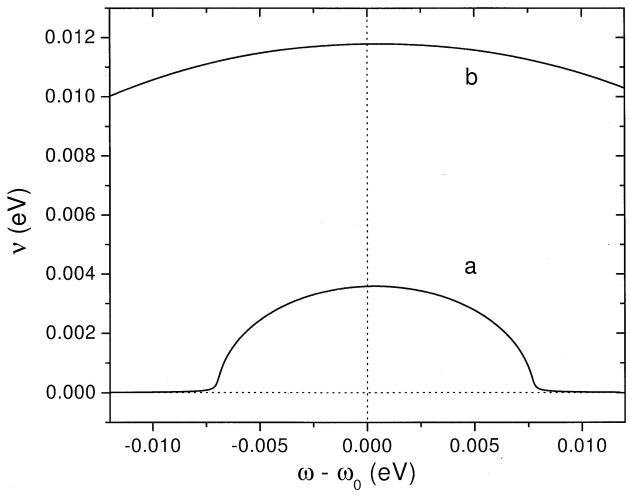

FIGURE 1. Frequency dependence of the surface-induced inhomogeneous damping $\nu = \nu_{n_e,n_h}(n)$ for the ground-state hh-exciton resonance ($n_e = 1$, $n_h = 1$, $n = 0$) of a GaAs quantum well of thickness $d = 60$ Å with (a) $Al_{0.3}Ga_{0.7}As$ barriers and (b) ideally infinite barriers.

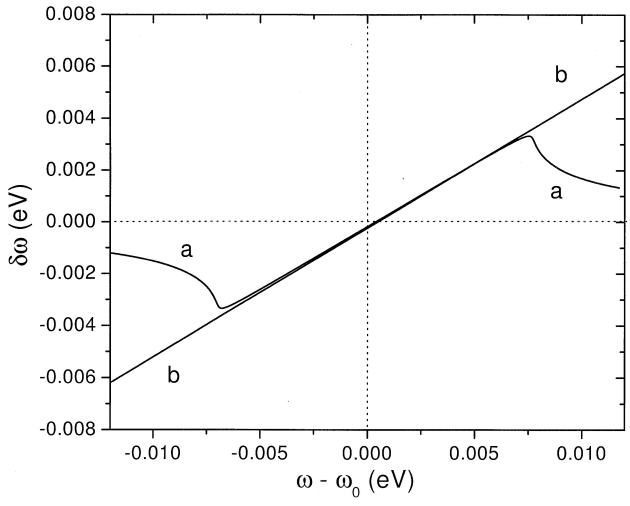

FIGURE 2. Frequency dependence of the surface-induced shift $\delta\omega$=$\delta\omega_{n_e,n_h}(n)$ for the ground-state hh-exciton resonance (n_e=1, n_h=1, n=0) of a GaAs quantum well of thickness $d = 60$ Å with (a) $Al_{0.3}Ga_{0.7}As$ barriers and (b) ideally infinite barriers.

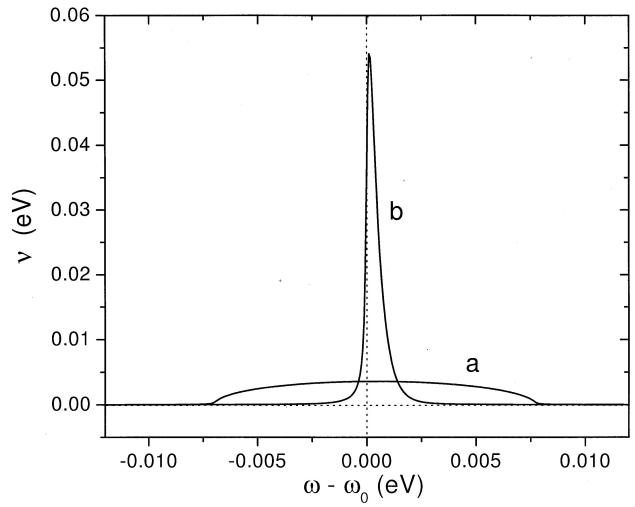

FIGURE 3. Frequency dependence of the surface-induced inhomogeneous damping ν=$\nu_{n_e,n_h}(n)$ for the ground-state hh-exciton resonance (n_e=1, n_h=1, n=0) of a GaAs quantum well of thickness d=60 Å with $Al_{0.3}Ga_{0.7}As$ barriers. Curves (a) and (b) were calculated by using the self-consistent approach (as in Fig. 1(a)) and the ordinary Born approximation, respectively.

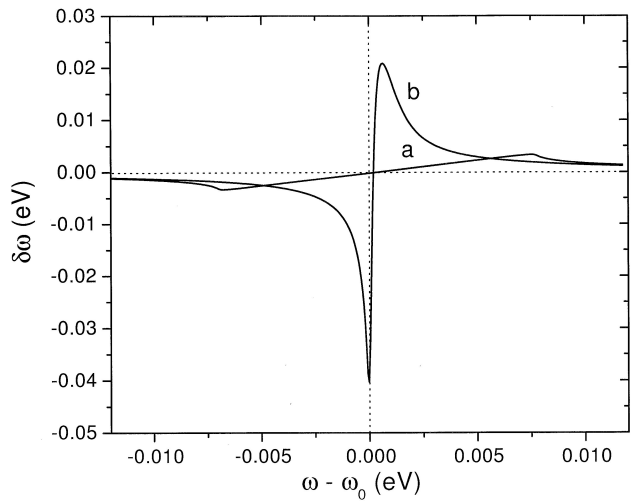

FIGURE 4. Frequency dependence of the surface-induced shift $\delta\omega$=$\delta\omega_{n_e,n_h}(n)$ for the ground-state hh-exciton resonance (n_e=1, n_h=1, n=0) of a GaAs quantum well of thickness d=60 Å with $Al_{0.3}Ga_{0.7}As$ barriers. Curves (a) and (b) were calculated by using the self-consistent approach (as in Fig. 2(a)) and the ordinary Born approximation, respectively.

to that caused by the damping ν, *i.e.* the resonance is broadened symmetrically. This effect of $\delta\omega$ on ν is clearly observed in the curve (a) of Fig. 1 and agrees with the asymptotic expressions (36) and (37). Note that the nonzero shift $\delta\omega$ at the resonance frequency ω_0 is negative with absolute value of the order of $\omega_W \ll \nu_{\max} = \nu_N$. Evidently, $\delta\omega(\omega_0) \to 0$ when $\omega_W \to 0$. For comparison purposes, we also present curve (b) that shows the shift $\delta\omega$ for the ideal case of infinite barriers (as in Fig. 1(b) for ν). It is seen that the behavior of $\delta\omega$ near the exciton resonance is practically the same for finite and infinite barriers. Only when the magnitude of the

resonance detuning $|\omega - \omega_0|$ is very large, the shift $\delta\omega$ is altered by the height of the potential barriers (see Fig. 2): the resonance shift is reduced in magnitude as the height of the potential barrier is diminished.

Let us compare our result, obtained within the self-consistent approach (curves (a) in Figs. 1–4), with the predictions of the ordinary Born approximation for the inhomogeneous broadening ν (Fig. 3(b)) and the shift $\delta\omega$ (Fig. 4(b)) of the ground-state exciton resonance for the GaAs quantum well with $Al_{0.3}Ga_{0.7}As$ barriers. Within the ordinary Born approximation the self-energy is given by Eq. (33) or Eq. (39) eliminating the action of $\mathcal{M}$ on itself, *i.e.* with $\mathcal{M}_{n_e n_h}(n) = 0$ in the denominator of the integrand therein. Hence, in this case, the line-shapes of $\nu(\omega)$ and $\delta\omega(\omega)$ are determined by the relation between ω_W and ν_0 alone. For the chosen parameters here, $\omega_W \approx \nu_0$ and the line-shape of $\nu(\omega)$ is primarily *asymmetric* and *sharp* (see Fig. 3(b)), unlike to the behavior predicted by the self-consistent approach (curve (a)). The *asymmetry* and *sharpness* of resonance in the ordinary Born approximation can also be observed in the shift $\delta\omega$ (see Fig. 4(b)). Note, as well, that in accordance with the estimation made in the previous section, the ordinary Born approach predicts extremely large values for both ν and $\delta\omega$ near the exciton resonance frequency ω_0. The latter result is, in practice, unrealistic for the case of weak exciton-surface scattering, and shows clearly the disadvantage of using the routine Born approach rather than the self-consistent one.

From the comparison of Fig. 1 (2) with 3 (4), we can conclude that the self-consistency leads to more substantial changes in the line-shape of the excitonic resonance than the height of the potential barriers does. We have also calculated spectra for ν and $\delta\omega$ for smaller values of $R_c (200\mathring{A} < R_c < 500\mathring{A})$, when the condition $\nu_0 < \omega_W$ is well satisfied and the surface disorder is still adiabatic. These calculations show that the line-shapes of $\nu(\omega)$ and $\delta\omega(\omega)$ are qualitatively the same as in Figs. 1–4.

Finally, it should be noted that according to the equation for the self energy $\mathcal{M}_{n_e n_h}(n)$ (39), [see also Eqs. (30) and (33)], the dependencies of the broadening $\nu_{n_e,n_h}(n)$ and shift $\delta\omega_{n_e,n_h}(n)$ on the resonance detuning $\omega - \omega_{n_e,n_h}(n)$ have the same form for all 2D-exciton n-th states with identical numbers n_e and n_h in a quantum well with adiabatic interface roughness. Therefore, for the GaAs quantum well considered above the spectra of $\nu_{1,1}(n)$ and $\delta\omega_{1,1}(n)$ with $n \neq 0$ for the hh-exciton are, respectively, as in curves (a) of Figs. 1–4, taking into account that only the quantity ω_0 should be replaced by $\omega_{1,1}(n)$.

6. Conclusion

We have developed a formalism for calculating the relaxation frequency ν and the shift $\delta\omega$ of exciton resonances in quasi-2D quantum wells with finite potential barriers and adiabatic surface disorder, *i.e.* with a correlation length R_c for the well width fluctuations much larger than the exciton radius a_0 ($R_c \gg a_0$). Our formalism was constructed on the basis of the self-consistent Green's function method and, consequently, it considers the inherent action of the exciton scattering on itself. Thanks to the adiabaticity of the surface disorder, we obtained relatively simple equations for the inhomogeneous broadening ν and shift $\delta\omega$ for all exciton resonances. We analyzed qualitatively these equations and discussed the condition of the transition from the quantum self-consistent limit to the classical one. Then we solved the equations for ν and $\delta\omega$ numerically for the specific case of a GaAs quantum well with $Al_{0.3}Ga_{0.7}As$ barriers. It was found that the self-consistency alters significantly the line-shape of exciton resonances, as it was compared with the predictions of the routine Born approximation. So, our results show that the relaxation frequency ν for ground-state hh-exciton resonance has a *broad*, almost *symmetric* maximum near the resonance frequency ω_0, whereas in the usual Born approach the resonance is *sharp* and *asymmetric*. On the other hand, the surface-induced resonance shift $\delta\omega$ vanishes near ω_0, and has different signs on the sides of the exciton resonance. The orders of magnitude of ν and $\delta\omega$ obtained within the self-consistent approach turned out to be more realistic than those predicted by the ordinary Born approximation.

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