Scaling of exciton binding energy and virial theorem in semiconductor quantum wells and wires

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Recent numerical calculations [F. Rossi, G. Goldoni, and E. Molinari, Phys. Rev. Lett. **78**, 3527 (1997)] have revealed a shape-independent hyperbolic scaling rule for the exciton binding energy versus the exciton Bohr radius in semiconductor quantum wires, and an enhancement in the exciton binding energy in a quantum wire with respect to a quantum well for a given exciton Bohr radius. These findings were attributed to the existence of a constant (shape- and/or size-independent) virial theorem value (potential- to kinetic-energy ratio), respectively, for the wires and wells, and its value was found to be larger (=4) for wires than (=2) for wells. In order to elucidate the physics underlying the above results, we reexamine this subject by calculating the exciton binding energy and the corresponding virial theorem value in quantum wells and wires with infinite confinement barriers. We find the following. (i) The virial theorem value is nonconstant but approaches 2 from above when reducing the finite extension of the electron and hole wave functions in the confined directions. This is because the origin of the virial theorem value of 2 lies in the inverse square Coulomb force being the only interaction seen by the electron and hole. (ii) The scaling rule is nonhyperbolic, because the virial theorem value is not a constant. (iii) The virial theorem value and the exciton binding energy are larger in a wire than in a well for a given exciton Bohr radius, because the wire exciton has a smaller kinetic energy in the nonconfined direction. (iv) The origin of the shape-independent scaling rule for wires lies in the close similarity of the effective Coulomb potentials for wires with different shapes and widths. The virial theorem value being or not being a constant is irrelevant to the scaling rule. (v) There exists a more fundamental and practically more useful shape-independent scaling rule. [S0163-1829(99)11803-4]

I. INTRODUCTION

Excitonic states in quantum wells and wires formed by semiconductor heterostructures have attracted great attention during the past three decades.[1] Various approaches have been used to calculate the exciton binding energy in these quasi-two-dimensional (2D) (Refs. 2–5) and quasi-one-dimensional (1D) structures.[6–9] Recently, Rossi, Goldoni, and Molinari[10] showed numerically that the scaling of the exciton binding energy (E_b) with the exciton Bohr radius ($a_{\rm ex}$) for quantum wires is independent of the shape of the wires, and that E_b is larger in a wire than in a well for a given $a_{\rm ex}$. They attributed these conclusions to their observation that the virial theorem value (potential- to kinetic-energy ratio) equaled 2 for wells (the same as that for a bulk isotropic exciton) and 4 for strongly confined wires, since $E_b=2(1+\langle K\rangle/\langle V\rangle)a_{\rm ex}^{-1}$ (where $\langle K\rangle$ and $\langle V\rangle$ are expectation values of kinetic and potential energy, respectively). Their finding of different (but constant) virial theorem values for wells and wires is puzzling, since a realistic wire will evolve into a well or the bulk as the confinement is gradually relaxed. It is also unclear as regards the reason why the virial theorem value in the well remains the same as that for the bulk while it changes abruptly to a larger value of 4 in the wire. In addition, it is important to know if these results are generic to reduced dimensionalities.

The purpose of this work is to explore the exciton scaling rule and the virial theorem in reduced dimensions in more detail. We observe that a shape-independent scaling rule does exist for quantum wires, but that the virial theorem value being or not being a constant is irrelevant. We show that the enhancement of the virial theorem value for the quantum wires studied in Ref. 10 is not intrinsic to the reduction in dimensionality, and the reason for the difference in the virial theorem value for the quantum well and wire lies in the difference in the effect of a finite extension of the exciton wave function in the confined direction(s) (due to nonzero well or wire width and/or finite barrier height) for different dimensionalities. The virial theorem value is not a constant for either wires or wells.

II. MODEL AND RESULTS

For simplicity, we assume a two-band model, that the barrier heights in wells and wires are infinite,[2,3,6–9] and the shapes or cross section of wires are either circular[7,9] or square.[6,8] We shall focus our analyses on wells and wires whose widths are smaller than the bulk exciton Bohr radius, so a frequently adopted approximation of neglecting the correlation between the confined and nonconfined directions[3,5,7–9] can be used to solve the exciton ground state in such wells and wires. The wave function for the exciton ground state is written as

$$\Psi_{\rm well}=\psi_e(z_e)\psi_h(z_h)\varphi(x,y) \tag{1}$$

for a quantum well and

$$\Psi_{\rm wire}=\psi_e(x_e,y_e)\psi_h(x_h,y_h)\varphi(z) \tag{2}$$

for a quantum wire, where ψ_e and ψ_h are the wave functions of the electron and hole confinement states, $x=x_e-x_h$, $y=y_e-y_h$, $z=z_e-z_h$, and $\varphi(x,y),\varphi(z)$ are the wave functions of exciton relative motion for the well and wire, respec-

tively. The confinement is chosen to be along the z direction for the well and in the x-y plane for the wire. The eigenvalue equation for the exciton is

$$\left\{-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V_{\text{well}}(x,y)\right\}\varphi(x,y)=-E_b\varphi(x,y) \quad (3)$$

for the well and

$$\left\{-\frac{\partial^2}{\partial z^2}+V_{\text{wire}}(z)\right\}\varphi(z)=-E_b\varphi(z) \quad (4)$$

for the wire, the units for the energy and length are $E_0=\mu e^4/(2\hbar^2\varepsilon_0^2)$ and $a_0=\hbar^2\varepsilon_0/(\mu e^2)$, μ is the exciton reduced mass in the nonconfined direction(s), and ε_0 is the dielectric constant. The effective 2D and 1D Coulomb potentials $V_{\text{well}}(x,y)$ and $V_{\text{wire}}(z)$ are defined as[5,9]

$$V_{\text{well}}(x,y)=-2\int\frac{|\psi_e(z_e)|^2|\psi_h(z_h)|^2}{\sqrt{x^2+y^2+(z_e-z_h)^2}}dz_e dz_h \quad (5)$$

and

$$V_{\text{wire}}(z)=-2\int\frac{|\psi_e(x_e,y_e)|^2|\psi_h(x_h,y_h)|^2}{\sqrt{(x_e-x_h)^2+(y_e-y_h)^2+z^2}}dx_e dy_e dx_h dy_h. \quad (6)$$

For the electron-hole relative motion described by Eq. (3) or Eq. (4), one can calculate the expectation values $\langle V\rangle=\langle\varphi|V_{\text{eff}}|\varphi\rangle$ and $\langle K\rangle=\langle\varphi|-\nabla^2|\varphi\rangle$ (where $V_{\text{eff}}=V_{\text{well}}$ or V_{wire}). Then, the virial theorem value is the ratio $-\langle V\rangle/\langle K\rangle$. As in Ref. 10, we define the exciton Bohr radius as

$$a_{\text{ex}}=\langle\Psi|r^{-1}|\Psi\rangle^{-1}, \quad (7)$$

where $r=\sqrt{x^2+y^2+z^2}$ and it follows that $a_{\text{ex}}=-2\langle V\rangle^{-1}$. Since a_{ex} depends only on the mean value rather than on the detailed features of the potential energy, it is logical to look for possible universal scaling rules using a_{ex} as a variable.

The effective potentials, Eqs. (5) and (6), for the well and wire are obtained numerically.[9,11] For the well, the variational wave function $\varphi(x,y)$ is assumed to have the form of a 2D hydrogenic wave function,[3,5] whereas for the wire, the eigenvalue equation is solved numerically. The effective potential for a circular wire can be expressed as[9]

$$V_{\text{wire}}^{\text{circular}}(z)=-\frac{2}{R}U_{\text{circular}}\left(\frac{z}{R}\right), \quad (8)$$

in E_0 and a_0 units, where R is the radius of the wire and U_{circular} is the ''universal potential'' defined in Ref. 9 for the circular wire. For a square wire with a width $2R$, one can similarly obtain a ''universal potential'' $U_{\text{square}}(z/R)$ and the corresponding effective potential $V_{\text{wire}}^{\text{square}}(z)$. Figure 1 shows a comparison of these two potentials. One observes that for the same value of R, $U_{\text{circular}}(0)>U_{\text{square}}(0)$, which occurs because the cross-section area of the circular wire $A_{\text{circular}}=\pi R^2$ is smaller than that of the square wire $A_{\text{square}}=4R^2$, and implies that the averaged electron-hole separation is smaller in the circular wire. Thus, for the same width R, the exciton binding energy is expected to be larger in the circular wire. However, we observe that for a square wire one can always find a smaller value of R that gives an effective potential whose magnitude is very close to that of a circular wire that has a specified value of R, as shown in Fig. 1. This is the primary reason for the shape-independent scaling rule.

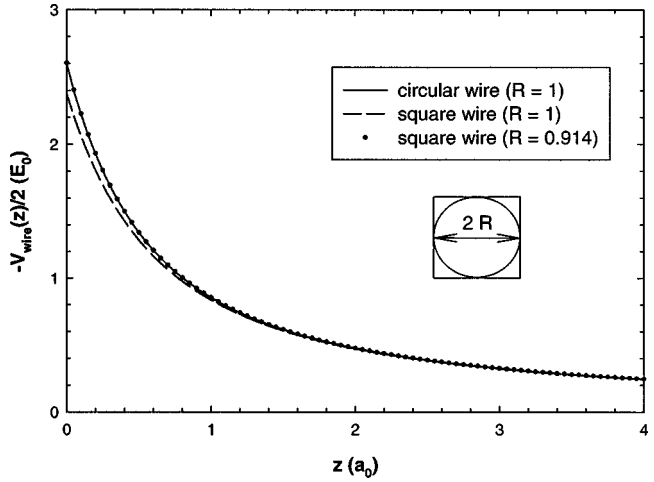

FIG. 1. Effective Coulomb potentials for circular and square quantum wires.

Figure 2 shows the exciton binding energy versus the exciton Bohr radius, where the different points correspond to values calculated for wells and circular and square wires of various widths. The two sets of data for circular and square wires lie almost on the same curve. Also shown in Fig. 2 are the results of the virial theorem value as a function of the exciton radius. Again, the two sets of data practically fall on the same curve. A more important observation is that the virial theorem value has a strong dependence on the exciton radius and approaches a value of 2 from above as the width of the well or wire approaches zero. The fundamental origin of the nonconstant virial theorem value lies in the coexistence of single-particle confinement potentials with the two-particle Coulomb interaction. Also, we would like to point out that an exact hyperbolic dependence and a constant virial theorem value of 2 occur in layer- and chain-type quasi-2D and quasi-1D semiconductors, where there is no such con-

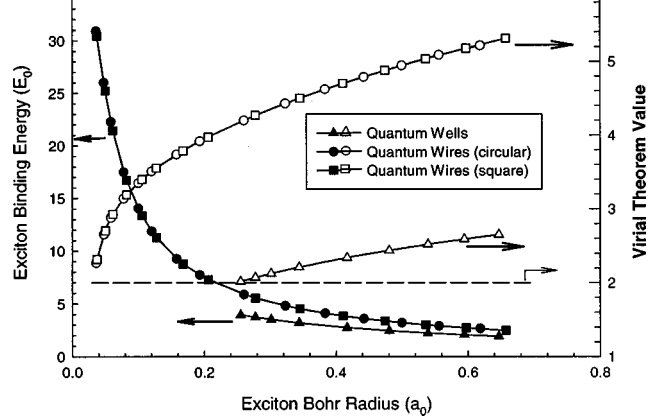

FIG. 2. Exciton binding energy and virial theorem value as a function of exciton Bohr radius in quantum wells, and circular and square quantum wires. The discrete points correspond to different well or wire widths. From left to right, the well widths (in a_0) are 0.01, 0.05, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, and 1.2; the wire widths are 0.02, 0.04, 0.06, 0.1, 0.15, 0.2, 0.3, and 0.4 to 1.8 in the 0.2 interval.

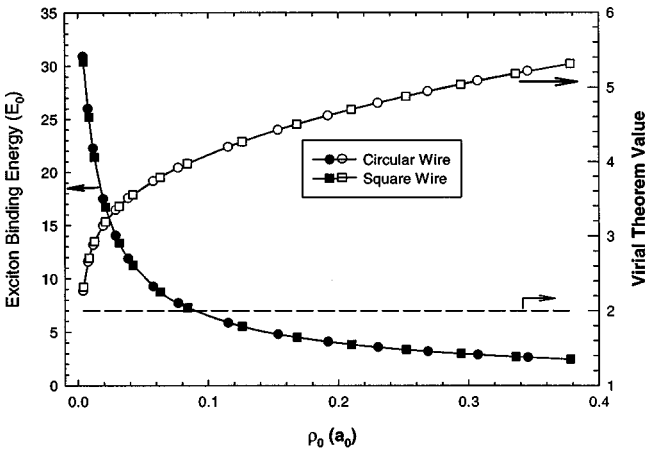

FIG. 3. Exciton binding energy and virial theorem value as a function of ρ_0 in circular and square quantum wires. The wire widths corresponding to the discrete points are the same as those in Fig. 2.

finement potential. More detailed discussions on these systems will be given in next section.

Another important finding is that a square wire of a half-width R_{square} is equivalent to a circular wire of a radius R_{circular}, when $R_{\text{square}}/R_{\text{circular}}=\rho_{0_{\text{circular}}}/\rho_{0_{\text{square}}}=\alpha$, where

$$\rho_0^{-1}\equiv\left\langle\frac{1}{\rho}\right\rangle\equiv\int\frac{|\psi_e(x_e,y_e)|^2|\psi_h(x_h,y_h)|^2}{\sqrt{(x_e-x_h)^2+(y_e-y_h)^2}}dx_e dy_e dx_h dy_h \tag{9}$$

and $\rho=\sqrt{x^2+y^2}$. In fact, $\alpha=U_{\text{square}}(0)/U_{\text{circular}}(0)=0.9136$. This ratio will of course be different for wires with different geometric shapes. Because of the above equivalence, we find a new shape-independent scaling rule: E_b versus ρ_0, as shown in Fig. 3. This new scaling rule is far more useful practically, because one only needs to know the single-particle states in order to calculate ρ_0.

III. DISCUSSIONS

A. Physical insights into the numerical results

The scaling rule given in Ref. 10, $E_b=\beta/a_{\text{ex}}$ (β being a constant), is essentially a plot of the exciton binding energy versus $\langle V\rangle^{-1}$, since $a_{\text{ex}}=-2\langle V\rangle^{-1}$. Thus, if the virial theorem value is a constant, as found for the structures calculated in Ref. 10, a hyperbolic scaling rule will be the trivial result. In Ref. 10, no physical reason was given for the value being constant and having the specific value equal to 4 for wires and 2 for wells. The physical origin of the virial theorem value of 2 for ideal 2D and 3D systems lies in the inverse square Coulomb force being the only interaction seen by the electron and hole. This apparently does not hold true in the presence of coexisting confinement potentials for the electron and hole. In fact, it has been pointed out earlier by Campi and Villavecchia[12] that in quantum wells the virial theorem value does not equal 2 any more except for the 2D limit, which is supportive of our result but contradicts that of Ref. 10. In an ideal 2D system, because the motion in the confined direction is completely inhibited, the inverse square force between the electron and hole is restored.

The deviation of the virial theorem value from 2 can be qualitatively understood from the following considerations. For an ideal 2D Coulomb interaction (zero well width), $V_{\text{2D}}(\rho)=-2/\rho$, if one employs a variational wave function $f(\rho)=\sqrt{2/(\pi\lambda^2)}\exp(-\rho/\lambda)$,[13] the expectation value of the kinetic energy is $\langle K\rangle=1/\lambda^2$, while the expectation value of the potential energy is $\langle V\rangle=-4/\lambda$. The virial theorem value equals 2 because $\lambda_0=0.5$ maximizes the binding energy. Since the effective 2D potential $|V_{\text{well}}(\rho)|<|V_{\text{2D}}(\rho)|$, a larger value of λ_0 is expected for a quantum well. Because of its $1/\lambda^2$ dependence, the kinetic energy decreases faster than the potential energy when plotted as a function of λ. Thus, a virial theorem value greater than 2 is expected for cases where the electron and hole wave functions have a finite extension in the confined direction, i.e., for finite well widths or finite barrier heights. For an ideal 1D Coulomb interaction (zero wire width), $V_{\text{1D}}(z)=-2/|z|$, and if the variational wave function $f(z)=\sqrt{1/\lambda}\exp(-|z|/\lambda)$ is used, we obtain $\langle K\rangle=1/\lambda^2$ and $\langle V\rangle=$ infinity. However, if we allow a small extension in the x-y plane, the Coulomb interaction $1/|z|$ is ''regularized'' to $1/(|z|+\delta)$,[14,9] where δ is a small positive number. For this regularized potential, $\langle V\rangle$ becomes finite, and the ratio $|\langle V\rangle 1/\langle K\rangle$ approaches 2 from above as δ approaches zero. On increasing δ or relaxing the confinement, the ratio increases. It is important to note that a larger virial theorem value does not necessarily imply a larger binding energy, since the binding energy is not maximized at the parameter value which gives the largest potential/kinetic energy ratio, and the exciton binding energy of the well or wire is not proportional to, but rather is inversely proportional to, the virial theorem value, as depicted in Fig. 2. The constant virial theorem value of 4 for wires found numerically in Ref. 10 is at least not a universal number for all wires. Recently, Thilagam[15] pointed out that having a constant virial theorem value of 4 is equivalent to having an effective 1D potential in the form of $1/\sqrt{z}$. However, such a potential is incorrect at two limits $z\rightarrow 0$ and ∞ (it should be finite at $z=0$ and approaches $1/z$ as $z\rightarrow\infty$).[9]

We have shown that there is indeed a shape-independent scaling rule for wires, even though the virial theorem value is not a constant. Its strong dependence on the exciton Bohr radius implies that the scaling rule is nonhyperbolic in general, although it was found to be hyperbolic for V- and T-shaped wires in Ref. 10. Thus, it appears inappropriate to attribute the existence of the scaling rule to the constant virial theorem value as in Ref. 10. The primary reason for the shape-independent scaling rule is that two wires which have different shapes and sizes can have very similar effective potentials, and thus turn out to have very similar exciton binding energies and Bohr radii.

The reason that the virial theorem value is larger in a wire than in a well for a given exciton Bohr radius is revealed by considering the definition of the exciton Bohr radius. If a_{ex} is used as a scaling variable for the virial theorem value, the difference in the virial theorem value for any two confined systems must originate in the difference in $\langle K\rangle$ for these systems (since $a_{\text{ex}}=-2\langle V\rangle^{-1}$ is fixed, $\langle V\rangle$ is the same for both systems). Figure 4 shows schematically the relative scale (qualitative) of the ground state exciton Bohr orbitals for bulk, well and wire systems for an equal value of the exciton Bohr radius a_{ex}. It is evident from Fig. 4 that for a given

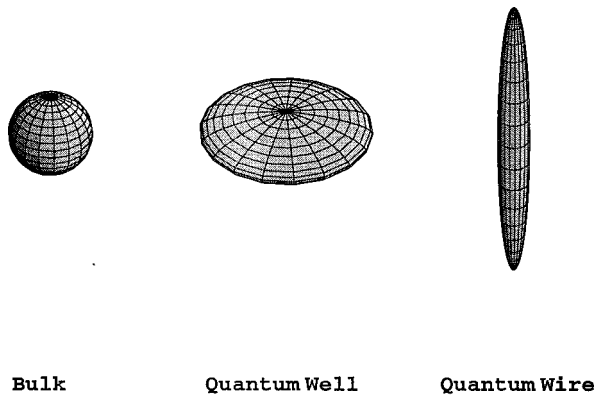

FIG. 4. A schematic qualitatively showing the relative scale of the ground-state exciton Bohr orbitals for bulk 3D, quantum-well (quasi-2D), and quantum-wire (quasi-1D) systems, for an equal value of the exciton Bohr radius a_{ex}.

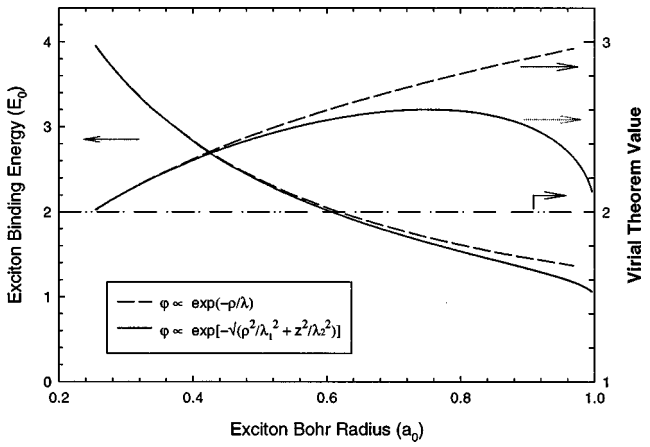

FIG. 5. Comparison of the exciton binding energy and virial theorem value as a function of exciton Bohr radius in quantum wells with and without considering the correlation effect. For the former, the well width varies from 0.01 to $10a_0$; for the latter, from 0.01 to $2.6a_0$.

value of a_{ex}, the average value of the electron-hole separation in the non-confined direction is largest for the wire and smallest for the bulk. Therefore, $\langle K\rangle$ will be largest in the bulk and smallest in the wire (because $\langle K\rangle$ is inversely proportional to the average electron-hole separation in the non-confined direction). Thus, for a given exciton Bohr radius, we expect a larger virial theorem value for the wire than for the well.

In Fig. 2, the virial theorem value increases monotonically with exciton Bohr radius for the wells and wires. However, we expect that it should eventually decrease to approach the 3D limit of 2 as $a_{\mathrm{ex}} \rightarrow a_0$ or the well or wire size $\rightarrow \infty$. The wave functions given by Eqs. (1) and (2) will never lead to the correct 3D limit, since the correlation between the confined and nonconfined directions has been ignored. Nevertheless, we expect that the results shown in Fig. 2 at least reveal the correct physical trend for these confined system. For quantum wells, the major difference between our work and that of Ref. 10 lies in the following three aspects: (i) the finite or infinite barrier height, (ii) the presence or absence of the correlation, and (iii) the use of a variational or a numerical technique. Since the barrier height will not cause a big change in the basic physics of interest to us (for instance, whether the virial theorem value is a constant equal to 2 or not), the first aspect could not be the reason for the qualitative difference between the result of Ref. 10 and ours or that of Ref. 12. In fact, the authors of Ref. 12 did not use the infinite barrier height assumption either. The correlation effect has been shown to be negligible for the region of small well width.[3] Also, the disagreement could not be due to the use of a variational technique, since the nonvariational approach of Ref. 12 yielded a conclusion qualitatively similar to ours. As regards the quantum wires, the correlation effect is expected to be even smaller in the more confined system (quantum wires) than in the quantum wells, and for this case our results are obtained numerically too. A final difference between our work and that of Ref. 10 lies in the aspect relating to the use of a realistic or an idealized geometric shape. It is important to note that the shape- and size-independent constant virial theorem value of 4 obtained in Ref. 10 does fall in the range of our result. If this value is indeed a constant for all those V- and T-shaped wires, the value of 4 could only be a fortuitous result, since there is nothing special about this number.

To show the validity of the approximate wave functions given by Eqs. (1) and (2) for the wells and wires in the region considered in Fig. 2, we examine the correlation effect in the less confined system—the quantum well. The correlation effect is included by generalizing $\varphi(x,y)$ in Eq. (1) to $\varphi(x,y,z)$. Accordingly, we define $\langle V\rangle = \langle \Psi_{\mathrm{well}} | -2/r | \Psi_{\mathrm{well}}\rangle$ and $\langle K\rangle = \langle H\rangle - \langle V\rangle - E_e - E_h$, where H is the total Hamiltonian and E_e and E_h are, respectively, the electron and hole binding energy. A frequently used trial function[3,12,16] is adopted,

$$\varphi(x,y,z) = \frac{N}{\sqrt{\pi \lambda_1^2 \lambda_2}} \exp\left(-\sqrt{\rho^2/\lambda_1^2 + z^2/\lambda_2^2}\right), \qquad (10)$$

where λ_1 and λ_2 are two variational parameters and N is the normalization constant. Figure 5 shows the exciton binding energy and virial theorem value as a function of exciton Bohr radius in quantum wells (with well width varying from 0.01 to $10a_0$). As expected, with increasing the exciton Bohr radius or the well width, the exciton binding energy approaches E_0 and the virial theorem value approaches the value of 2 for the bulk isotropic exciton.

B. Scaling rule and virial theorem value in layers and chain-type semiconductors

Layer and chain-type semiconductors represent another category of quasi-2D and -1D systems.[17] For these type of semiconductors, excitonic states can be modeled very well by a simple effective-mass theory with anisotropy in both the mass and dielectric constant.[18–20] A model Hamiltonian for an anisotropic exciton with uniaxial symmetry can be written as[21]

$$\left\{ -\frac{\hbar^2}{2\mu_\perp}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2\mu_\parallel}\frac{\partial^2}{\partial z^2} - \frac{e^2}{\sqrt{\varepsilon_\perp \epsilon_\parallel (x^2+y^2) + \varepsilon_\perp^2 z^2}} \right\} \psi = E\psi, \qquad (11)$$

where $\mu_\perp(\varepsilon_\perp)$ and $\mu_\parallel(\varepsilon_\parallel)$ are exciton reduced masses (dielectric constants) in the directions perpendicular and parallel to the uniaxis, respectively.

Since the potential in the above equation satisfies the relation $\langle \mathbf{r}\cdot\nabla V\rangle = -\langle V\rangle$, because of the generalized virial theorem $2\langle K\rangle = \langle \mathbf{r}\cdot\nabla V\rangle$,[22] the virial theorem $2\langle K\rangle = -\langle V\rangle$ still holds true for these quasi-2D and -1D systems. Thus, the exciton binding energy scales as $E_b = a_{\mathrm{ex}}^{-1}$. The major difference between semiconductor quantum well or wire and the layer or chain-type semiconductors is that the former have a long-range confinement potential while the latter do not.

C. Scaling rule and virial theorem value in short-period semiconductor superlattices

For semiconductor superlattices with a period $d \ll (m^* V_0/\hbar^2)^{-1/2}$ such that the dispersion along the superlattice axis is nearly parabolic, Ivchenko and Pikus pointed out[23] that the exciton binding energy can be obtained by solving Eq. (11). Thus, the scaling rule and the virial theorem value for the short-period superlattices are the same as those in the layer and chain-type semiconductors.

IV. SUMMARY

In summary, we have studied the scaling rule for exciton binding energy versus exciton Bohr radius and the virial theorem value in semiconductor quantum wells and wires, and compared them to closely related systems: layer and chain-type semiconductors and short-period semiconductor superlattices. While there is indeed a shape-independent scaling rule for exciton binding energies in semiconductor quantum wires, as observed in Ref. 10, we have found more general properties regarding the scaling rule and the related virial theorem value in wells and wires, and provided physical insights into these properties.

In general, the scaling rule is nonhyperbolic and the virial theorem value is nonconstant. The deviation from hyperbolic behavior is directly associated with the virial theorem value being nonconstant, and the reason for the virial theorem value being nonconstant and greater than 2 is the finite extension of the exciton wave function in the confined directions. Because the wire exciton has a smaller kinetic energy in the nonconfined direction, for a given exciton Bohr radius, the virial theorem value and exciton binding energy are larger in the wire than in the well. The shape-independent scaling rule for quantum wires occurs because the effective potentials for wires with different shapes can be approximately made equivalent to that for wires with a specifically chosen shape but with different widths. A shape-independent scaling rule that does not require directly solving the exciton equation is proposed.

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