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Linewidths of electron-impurity resonant states in semiconductor quantum wells

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Giant Interactions in Rydberg Systems (GiRyd)

Pavel A. Belov
Universität Rostock
(pavelbelov@gmail.com)

25th European Conference on Few-Body Problems in Physics
August 1, 2023

Excitons in bulk semiconductor

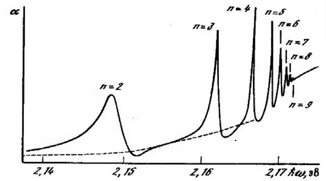
$$H_X = -\frac{\hbar^2}{2m_e}\Delta_{\vec{r}_e} - \frac{\hbar^2}{2m_h}\Delta_{\vec{r}_h} - \frac{e^2}{\epsilon|\vec{r}_e - \vec{r}_h|}$$

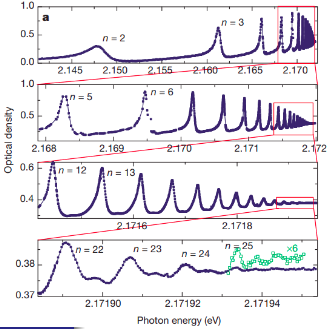
where m_e and m_h are effective masses

$$E_X \sim -\frac{\mathrm{Ry}}{N^2}$$

where for semiconductors, the exciton Rydber

$$\mathrm{Ry} = \frac{\mu e^4}{2\hbar^2\epsilon^2} \sim 10 - 100 \text{ meV}$$





The exciton was discovered in bulk Cu_2O semiconductor by E. F. Gross and N. A. Karryev at the Ioffe Institute (Leningrad) in 1952

Renaissance at TU Dortmund in 2014!

Exciton in quantum well (as exemplified by GaAs)

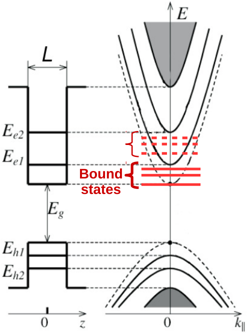
- Electron in QW: $\frac{\mathbf{k}_e^2}{2m_e} + V_e(z_e)$
- Hole in QW: $\frac{\mathbf{k}_h^2}{2m_h} + V_h(z_h)$
- Quantization: $E_n \sim \frac{\hbar^2}{2m_{e,h}} \left(\frac{\pi\, n_{e,h}}{L}\right)^2$
- Attractive Coulomb potential:

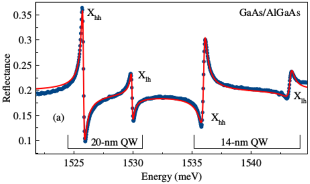
$$-\frac{e^2}{\epsilon|\mathbf{r}_e - \mathbf{r}_h|}$$

The bound and quasibound states appear below subbands

The bound e-h states are EXCITON states

For more details:
E.L. Ivchenko Optical Spectroscopy of Semiconductor Nanostructures (2005).
E.S. Khramtsov J. Appl. Phys. 119 (2016) 184301





Two-band Schrödinger equation for exciton in QW

$$\left(-\frac{\hbar^2}{2m_e}\Delta_{\vec{r}_e} - \frac{\hbar^2}{2m_{hh}}\Delta_{\vec{r}_h} - \frac{e^2}{\epsilon|\vec{r}_e - \vec{r}_h|} + V_e(z_e) + V_h(z_h)\right)\Psi = E_X\Psi$$

Separation of the center-of-mass motion in the QW plane

Introduce coordinate of center-of-mass motion (X, Y), relative motion (x, y) and radius in QW plane: $\rho = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2}$
Look for s-wave solution in the following form (magnetic q.n. $m = 0$):

$$\Psi(X, Y, x, y, z_e, z_h) = \frac{\psi(\rho, z_e, z_h)}{\rho} \exp(iK_x X) \exp(iK_y Y) \exp(im\phi)$$

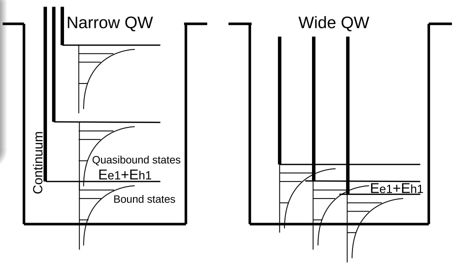
$$\left(K - \frac{e^2}{\epsilon\sqrt{\rho^2 + (z_e - z_h)^2}} + V_e(z_e) + V_h(z_h)\right)\psi(\rho, z_e, z_h) = E\psi(\rho, z_e, z_h)$$

$$K = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_{hh}}\frac{\partial^2}{\partial z_h^2} - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\right)$$

$$\left(H_e(z_e)+H_h(z_h)-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}-\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\right)-\frac{e^2}{\epsilon\sqrt{\rho^2+(z_e-z_h)^2}}\right)\psi(\rho,z_e,z_h)=E\psi(\rho,z_e,z_h)$$

Energy of exciton states: $E < E_{e1} + E_{h1}$

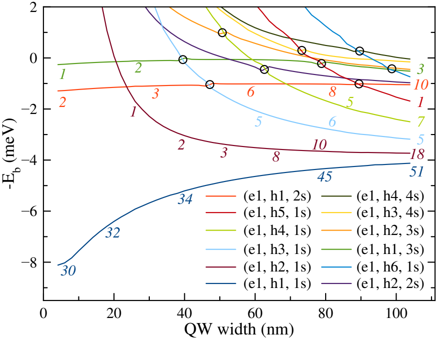
- The lower boundary of the continuous spectrum is $E_{e1} + E_{h1}$.
- As QW width increases, the energy levels of excited quantum-confined states "drop down" from continuum to discrete part of spectrum

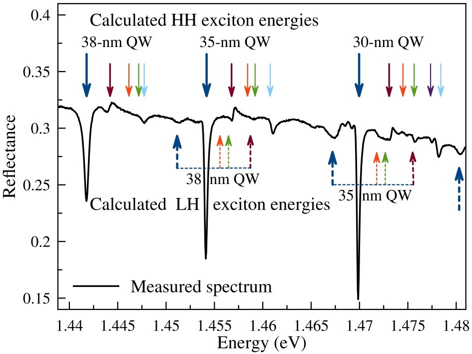


- The thresholds $E_{ei} + E_{hj}$ of energies of QW eigenmodes are denoted by long horizontal lines.
- For the wide QWs the different branches of the Coulomb spectrum are shifted horizontally for visiability.
- P. A. Belov, Phys. E 112 (2019) 96

Electron-hole energy levels
for narrow QW, for wide QW.

The reflectance spectrum of the heterostructure with three single $In_xGa_{1-x}As/GaAs$ QWs for $x \leqslant 0.08$



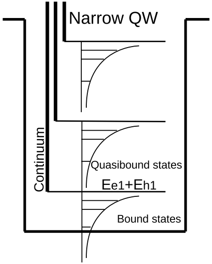


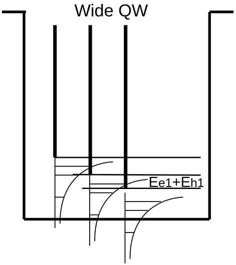
Calculated energies of heavy-hole exciton (arrows) and light-hole exciton (dashed arrows) in $In_{0.09}Ga_{0.91}As/GaAs$ QW

Resonant states of *eh* pairs in semiconductor QWs

$$\left(H_e(z_e)+H_h(z_h)-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}-\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\right)-\frac{e^2}{\epsilon\sqrt{\rho^2+(z_e-z_h)^2}}\right)\psi(\rho,z_e,z_h)=E\psi(\rho,z_e,z_h)$$

Resonant states: $E > E_{e1} + E_{h1}$





The linewidth brodening of resonant eh states is important
however more difficult to estimate due to square-unintegrable wave function

Linewidth broadening $\hbar\Gamma$ by the complex scaling

Exterior rotation of the variables >0 (<0) into upper(lower) complex half-plane by angle θ

$$\rho \to R(\rho)$$

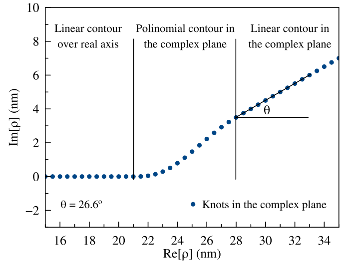
$$R(\rho) = \begin{cases} \rho & \rho < \rho_0 \\ \rho_0 + (\rho - \rho_0)\exp i\theta & \rho \geqslant \rho_0 \end{cases}$$

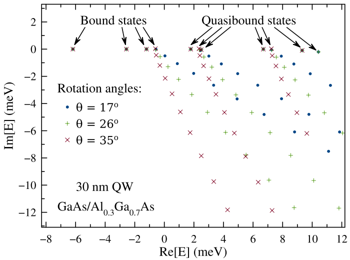
Then, the second partial derivative over R is expressed as

$$\frac{\partial^2}{\partial R^2} = \frac{1}{(R'_\rho)^2}\frac{\partial^2}{\partial \rho^2} - \frac{R''_\rho}{(R'_\rho)^3}\frac{\partial}{\partial \rho}.$$

Solve the non-Hermitian eigenvalue problem for $E - i\hbar\Gamma$.

We can identify the quasibound states (resonances) in the continuum and determine nonradiative broadening $\hbar\Gamma$.





Linewidth broadening of *eh* resonant states in QWs

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}\right) - \frac{e^2}{\epsilon\sqrt{\rho^2+z^2}}\right] - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial Z^2} + V_e(z_e)+V_h(z_h)$$

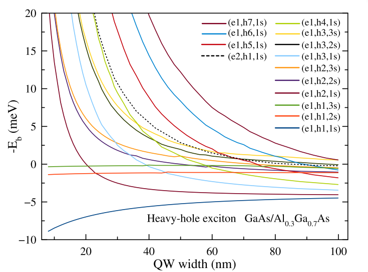
- For GaAs, broadening $\hbar\Gamma$ is defined by electron eigenmodes: Much stronger coupling of electron to continuum.
- The reduced mass is $\mu \sim m_e$
- Linear dependence on QW width:

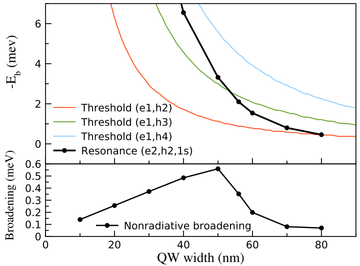
$$\hbar\Gamma(L) \sim L$$

Disagreement with the Fano theory of resonances:

$$\hbar\Gamma(L) \sim L^4$$

B. Monozon, P. Schmelcher, PRB, 2005.





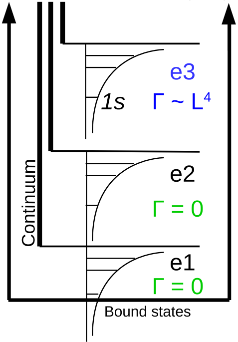
$\hbar\Gamma(L)$ of electron-impurity resonant states in QWs

The Hamiltonian is similar, but more simple:

$$\left[-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z^2}+V_e(z)\right]-\frac{e^2}{\epsilon\sqrt{\rho^2+z^2}}$$

$$-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}\right)$$

Monozon and Schmelcher (2005)

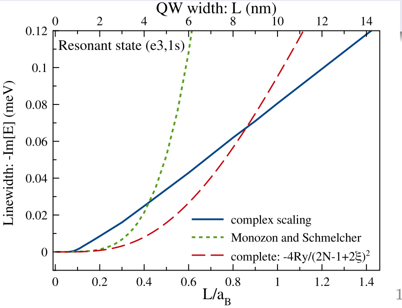


- Fano prediction for linewidth:

$$\Gamma = C\frac{\mathrm{Ry}}{(2N-1)^3}\left(\frac{L}{a_B}\right)^4, \quad L \ll a_B$$

Our calculations for $e3$ subband give:

$$\Gamma \sim L^1, \quad L \sim a_B$$



$\hbar\Gamma(L)$ of electron-impurity resonant states in QWs

The Hamiltonian is similar, but more simple:

$$\left[-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z^2}+V_e(z)\right]-\frac{e^2}{\epsilon\sqrt{\rho^2+z^2}}$$
$$-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}\right)$$

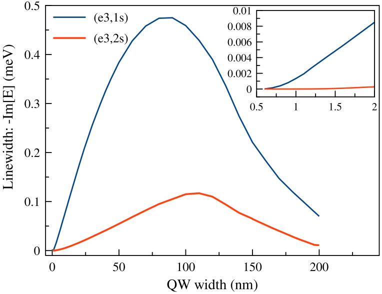
- Our complex-scaling calculations show linear dependence on QW linewidth:

$$\hbar\Gamma(L)\sim L,\qquad L\sim a_B$$

- For very narrow QWs (~ 1 nm), Fano theory works:

$$\hbar\Gamma(L)\sim L^4,\qquad L\ll a_B$$

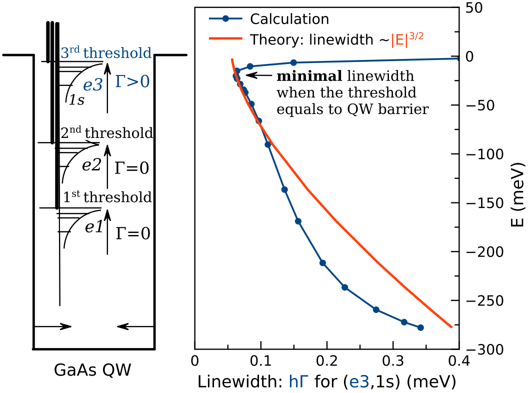
Our complex scaling calculations: (P. Belov, PRB, 2022)



The infinite-barrier QWs are studied.

P. A. Belov, PRB 105 (2022) 155417

The linewidth of a resonance state in finite-barrier QW



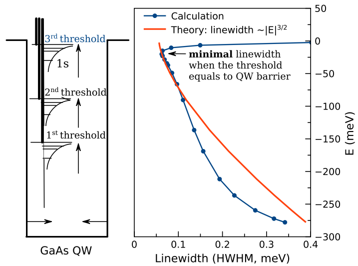
- Coulomb-like series of $e3$ subband has nonzero linewidth $\Gamma > 0$
- In spite of the finite barrier, the linewidth $\to 0$ as $L \to 0$.
- The linewidth is gradually decreasing until Coulomb threshold reaches QW barrier
- Theory (Zel'dovich 1971) predicts:

$$\hbar\Gamma \sim E^{3/2}$$

The minimal resonance width is achieved when Coulomb threshold of $e3$ subband reaches QW barrier

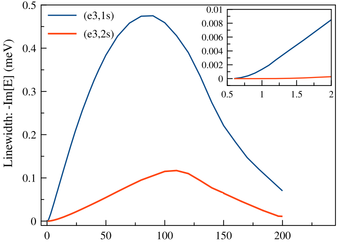
Conclusion

- The semiconductor structures with QW can be grown
- The spectrum of excitons in QWs can be calculated
- The linewidths of resonant *eh* and electron-impurity states can be estimated by the complex scaling
- The numerics improves and extends theoretical predictions



Presented results can be found in
P. A. Belov, PRB 105, 155417 (2022)
P. A. Belov, Physica E 112, 96 (2019)

pavelbelov@gmail.com



Other publications:
J. Appl. Phys. 119, 184301 (2016)
J. Phys. Conf. Ser. 1199, 012018 (2018)
Phys. Rev. Res. 2, 033510 (2020)

Batumi, Georgia

Thank you for your attention!