Perturbation theory schemes for analysis of spheroidal quantum dot models in adiabatic approximation

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OUTLINE

- Problems. In effective mass approximation for electronic (hole) states of spheroidal quantum dots under influence of the homogeneous electric field the boundary-value problems are formulated in the framework of Kantorovich and adiabatic methods.

- Methods. The different perturbation theory schemes are derived by using sets of adiabatic basis functions given in analytical form.

- Results. Comparative analysis of eigenvalues and eigenfunctions of the problem is presented based on both numerical and analytical methods.

- Applications Calculations of absorption coefficient of ensembles of spheroidal quantum dots in the homogeneous electric fields.

Problem

Spectral and optical characteristics of models of bulk semiconductor and low dimensional semiconductor nanostructures: quantum wells(QWs), quantum wires(QWrs) and quantum dots(QDs)

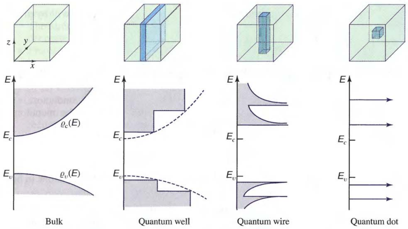


Figure 16.1-29 The density of states in different confinement configurations. The conduction and valence bands split into overlapping subbands that become successively narrower as the electron motion is restricted in a greater number of dimensions.

from B.E.A. Saleh M.C. Teich, Fundamentals of photonics (Wiley, 2007)

J. Phys. D: Appl. Phys. **41** (2008) 162004 Fast Track Communication

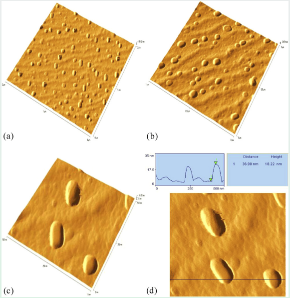


Figure 1. AFM views of LPE grown InAsSbP unencapsulated QDs on InAs(1 0 0) substrate: (*a*) oblique $S = 2 \times 2\,\mu m^2$, (*b*) oblique $S = 1 \times 1\,\mu m^2$, (*c*) oblique $S = 500 \times 500\,nm^2$ and (*d*) plane.

from K.M. Gambaryan et al J. Phys. D **41**, 162004 (2008)

Application of Quantum dots:

High performance transistors and lasers

Quantum dot technology is one of the most promising candidates for use in solid-state quantum computation.

Setting equations

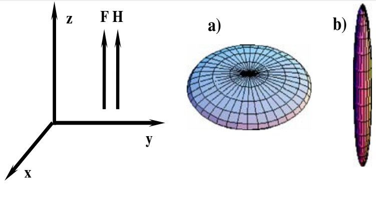


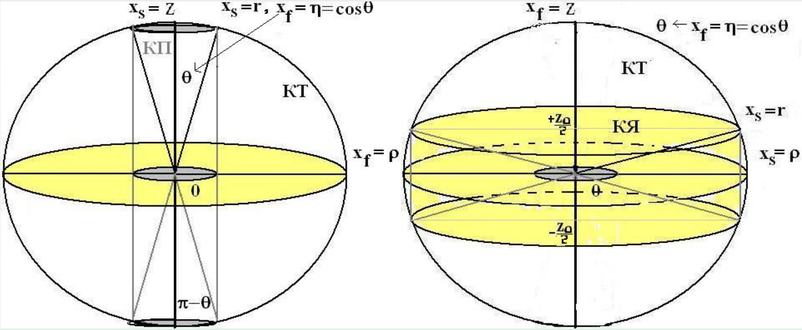
Fig. 1 (**a**) Strongly oblate ellipsoidal quantum dot. (**b**) Strongly prolate ellipsoidal quantum dot

In the effective mass approximation of the $\vec{k}\cdot\vec{p}$ theory the Schrödinger equation for the slow varying envelope function $\Psi(\vec{r}) \equiv \Psi^{e(h)}(\vec{r})$ of an impurity electron (e) or hole (h) under the influence of a uniform magnetic field $\vec{H}$ with vector-potential $\vec{A} = \frac{1}{2}\vec{H} \times \vec{r}$ and electric field $\vec{F}$ in QD, QW, or QWr reads as

$$\left\{ \frac{1}{2\mu}\left(\hat{\vec{p}} - \frac{q_1}{c}\vec{A}\right)^2 + q_1(\vec{F}\cdot\vec{r}) + U_{conf}(\vec{r}) - \frac{q}{\kappa|\vec{r}|} - E \right\} \Psi(\vec{r}) = 0,$$

Here $\vec{r}$ is the radius-vector, $|\vec{r}| = \sqrt{x^2 + y^2 + z^2}$,
$q = q_1 q_2 e$, where $q_1 = \pm e$ and $q_2 e$ are the Coulomb charges of the electron (hole) and the impurity center, κ is the dc permittivity,
$U_{conf}(\vec{r})$ is infinite or finite (Woods-Saxon) well confinement potential
$\mu = \beta m_e$ is the effective mass of the electron or hole and reduced atomic units (for example, in GaAs $q = 1, \kappa = 13.18$, $\beta_e = 0,067, \beta_h = \beta_e/0.12$), $a_e = (\kappa/\beta_e)a_B = 102$Å, $E_e = (\beta_e/\kappa^2)Ry = 5.2$ meV, $a_h = 15$Å, $E_h = (\beta_h/\kappa^2)Ry = 49$ meV, $\gamma = H/H_0^*$, $H_0^* = 6$T, $\gamma_F = F/F_0^*$, $F_0 = 133$kV/cm).

Fast and slow variables for QD, QWr and QW models



Systems of cylindrical (z, ρ, φ) and spherical $(r, \eta = \cos\theta, \varphi)$ coordinates(at shift $z_c = 0$): (a) for QD, QWr and (a) for QD, QW and their correspondence to fast x_f and slow x_s variables.

Comment. One can see that in cylindrical coordinates: a) for QD, QWr $x_f = \rho$, $x_s = z$, b) for QD, QW $x_f = z$, $x_s = \rho$, i.e. fast and slow variables are changed places. In spherical coordinates for QD, QW and QWr fast $x_f = \eta$ and slow $x_s = r$ variables are the same.

	CC		SC
	OSQD	PSQD	SQD
x_f	z	ρ	η
x_s	ρ	z	r
g_{1f}	1	ρ	1
g_{2f}	1	ρ	$1-\eta^2$
g_{1s}	ρ	1	r^2
g_{2s}	ρ	1	r^2
g_{3s}	1	1	r^2

Close-coupling and Kantorovich (Adiabatic) methods

The Schrödinger equation reads as

$$\left(\frac{1}{g_{3s}(x_s)}\hat{H}_2(x_f;x_s)+\hat{H}_1(x_s)+\hat{V}_{fs}(x_f,x_s)-2E\right)\Psi(x_f,x_s)=0,$$

$$\hat{H}_2=-\frac{1}{g_{1f}(x_f)}\frac{\partial}{\partial x_f}g_{2f}(x_f)\frac{\partial}{\partial x_f}+\hat{V}_f(x_f;x_s),$$

$$\hat{H}_1=-\frac{1}{g_{1s}(x_s)}\frac{\partial}{\partial x_s}g_{2s}(x_s)\frac{\partial}{\partial x_s}+\hat{V}_s(x_s).$$

$\hat{H}_2(x_f;x_s)$ is the Hamiltonian of the fast subsystem,

$\hat{H}_1(x_s)$ is the Hamiltonian of the slow subsystem,

$V_{fs}(x_f,x_s)$ is interaction potential.
The Kantorovich expansion of the desired solution of BVP:

$$\Psi(x_f,x_s)=\sum_{j=1}^{j_{\max}}\Phi_j(x_f;x_s)\chi_j(x_s).$$

BVP for fast subsystem

The equation for the basis functions of the fast variable x_f and the potential curves, $E_i(x_s)$ continuously depend on the slow variable x_s as a parameter

$$\left\{\hat{H}_2(x_f;x_s) - E_i(x_s)\right\}\Phi_i(x_f;x_s) = 0,$$

The boundary conditions at $x_f^b(x_s)$, $b = \min, \max$

$$\lim_{x_f \to x_f^b(x_s)} \left(N_f(x_s)g_{2f}(x_s)\frac{d\Phi_j(x_f;x_s)}{dx_f} + D_f(x_s)\Phi_j(x_f;x_s)\right) = 0.$$

The normalization condition

$$\langle\Phi_i|\Phi_j\rangle = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)\Phi_j(x_f;x_s)g_{1f}(x_f)dx_f = \delta_{ij}.$$

BVP for slow subsystem

The effective potential matrices of dimension $j_{\max} \times j_{\max}$:

$$U_{ij}(x_s) = \frac{1}{g_{3s}(x_s)}\hat{E}_i(x_s)\delta_{ij} + \frac{g_{2s}(x_s)}{g_{1s}(x_s)}W_{ij}(x_s) + V_{ij}(x_s),$$

$$V_{ij}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)V_{fs}(x_f,x_s)\Phi_j(x_f;x_s)g_{1f}(x_f)dx_f,$$

$$W_{ij}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \frac{\partial\Phi_i(x_f;x_s)}{\partial x_s}\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}g_{1f}(x_f)dx_f,$$

$$Q_{ij}(x_s) = -\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}g_{1f}(x_f)dx_f.$$

BVP for slow subsystem

The SDE for the slow subsystem (the adiabatic approximation is a diagonal approximation for the set of ODEs)

$$\mathbf{H}\chi^{(i)}(x_s) = 2E_i\,\mathbf{I}\chi^{(i)}(x_s),$$

$$\mathbf{H} = -\frac{1}{g_{1s}(x_s)}\mathbf{I}\frac{d}{dx_s}g_{2s}(x_s)\frac{d}{dx_s} + \hat{V}_s(x_s)\mathbf{I} + \mathbf{U}(x_s) + \frac{g_{2s}(x_s)}{g_{1s}(x_s)}\mathbf{Q}(x_s)\frac{d}{dx_s} + \frac{1}{g_{1s}(x_s)}\frac{dg_{2s}(x_s)\mathbf{Q}(z)}{dx_s},$$

with the boundary conditions at x_s^b, $b = \min, \max$

$$\lim_{x_s \to x_s^b}\left(N_s g_{2s}(x_s)\frac{d\chi(x_s)}{dx_s} + D_s\chi(x_s)\right) = 0.$$

Basis functions and effective potentials

For oblate spheroidal QDs ($x_f = z$, $x_s = \rho$) with impenetrable walls

$$B_i\left(x_f; x_s\right) = B_i^{\sigma}\left(x_f; x_s\right) = \sqrt{\frac{a}{c\sqrt{a^2 - x_s^2}}} \sin\left(\frac{\pi n_o}{2}\left(\frac{x_f}{c\sqrt{1 - x_s^2/a^2}} - 1\right)\right),$$

$$E_i(x_s) = E_i^{\sigma}(x_s) = E_{i;0}\frac{a^2}{(a^2 - x_s^2)}, \quad E_{i;0} = \frac{\pi^2 i^2}{4c^2}, \quad U_{ii}(x_s) = 0,$$

$$U_{ij}(x_s) = U_{ij;0}(x_s)\frac{\sqrt{a^2 - x_s^2}}{a}, \quad U_{ij;0}(x_s) = \frac{8\gamma_F cij(-1 + (-1)^{i+j})}{(i^2 - j^2)^2\pi^2},$$

$$H_{ii}(x_s) = H_{ii;0}(x_s)\frac{a^2 x_s^2}{(a^2 - x_s^2)^2}, \quad H_{ii;0}(x_s) = \frac{3 + \pi^2 i^2}{12a^2},$$

$$H_{ij}(x_s) = H_{ij;0}(x_s)\frac{a^2 x_s^2}{(a^2 - x_s^2)^2}, \quad H_{ij;0}(x_s) = \frac{2ij(i^2 + j^2)(1 + (-1)^{i+j})}{a^2(i^2 - j^2)^2},$$

$$Q_{ij}(x_s) = Q_{ij;0}(x_s)\frac{a x_s}{a^2 - x_s^2}, \quad Q_{ij;0}(x_s) = \frac{ij(1 + (-1)^{i+j})}{a(i^2 - j^2)}, \quad j \neq i.$$

The convergence of eigenenergy $\mathcal{E}_t$ vs number $j_{\max}$ of basis functions at $\gamma_F = 0$.

Fast and slow variables $x_f = z$ and $x_s = \rho$ (*oblate* SQD and spherical QD), number of nodes $i = (n_{zo} = n_o - 1, n_{\rho o})$, * notes diagonal approximation at $j = 2$

$j_{\max}$	$a = 2.5$, $c = 0.5$			$a = 2.5$, $c = 2.5$		
i	(0,0)	(0,1)	(2,0)	(0,0)	(0,1)	(2,0)
C	12.737 41	19.936 21	96.696 83*	1.468 496	5.445 665*	5.589 461
1	12.765 48	20.046 02	96.753 17*	1.590 238	5.766 612*	6.004 794
2	12.764 90	20.041 33	96.754 27	1.580 243	5.340 214	6.329 334
4	12.764 82	20.040 74	96.752 15	1.579 273	5.316 872	6.317 204
16	12.764 81	20.040 65	96.752 01	1.579 140	5.314 832	6.316 562
Exact				1.579 136	5.314 793	6.316 546

Fast and slow variables $x_f = \rho$ and $x_s = z$ (*prolate* SQD and spherical QD), number of nodes $i = (n_{\rho p}, n_{zp})$, * notes diagonal approximation at $j = 2$

$j_{\max}$	$c = 2.5$, $a = 0.5$			$c = 2.5$, $a = 2.5$		
i	(0,0)	(0,2)	(1,0)	(0,0)	(0,2)	(1,0)
C	25.184 73	34.428 85	126.424 5*	1.493 612	5.131 784	5.898 668*
1	25.201 74	34.530 30	126.456 5*	1.584 433	5.680 831	6.071 435*
2	25.201 29	34.525 78	126.457 3	1.579 860	5.331 101	6.324 717
4	25.201 21	34.525 12	126.456 1	1.579 239	5.316 732	6.317 058
16	25.201 20	34.525 02	126.456 1	1.579 138	5.314 828	6.316 554
Exact				1.579 136	5.314 793	6.316 546

The Lennard-Jones perturbation theory[1] in nondiagonal adiabatic approximation

We expand the above effective potentials of **the BVP for slow subsystem** in Taylor series in a vicinity of $x_s = 0$:

$$E_i(x_s) = E_{i;0} + \sum_{k=1}^{k_{\max}} \frac{E_{i;0}}{\tau^{2k}} x_s^{2k}, \quad U_{ij}(x_s) = U_{ij;0} + \sum_{k=1}^{k_{\max}} \frac{\tilde{U}_{ij;k}}{\tau^{2k}} x_s^{2k},$$

$$H_{ij}(x_s) = \sum_{k=1}^{k_{\max}} k \frac{H_{ij;0}}{\tau^{2k}} x_s^{2k}, Q_{ij}(x_s) = \sum_{k=1}^{k_{\max}} \frac{Q_{ij;0}}{\tau^{2k-1}} x_s^{2k-1},$$

where $\tilde{U}_{ij;k} = \frac{(2k-3)!!}{(2k)!!} U_{ij;0}$ and parameter τ equals $\tau = a$ for OSQD, and $\tau = c$ for PSQD.

[1] N. Mott and I. Sneddon, *Wave Mechanics and its Applications* (Clarendon, Oxford, 1948).

The Lennard-Jones perturbation theory

It leads to the BVP for a set of ODEs of slow subsystem with respect to the unknown vector functions $\chi_t(x_s) = (\chi_{1;t}(x_s), ..., \chi_{j_{\max};t}(x_s))^T$ corresponded to unknown eigenvalues $2E_t \equiv \mathcal{E}_t$:

$$\left(\mathrm{D}^{(0)} + (E_{i;0} - \mathcal{E}_t) + \check{V}_s(x_s) + \sum_{k=1}^{k_{\max}} \frac{E_{i;0} + kH_{ii;0}}{\tau^{2k}} x_s^{2k} \right) \chi_{i;t}(x_s)$$

$$+ \sum_{j \neq i}^{j_{\max}} \sum_{k=1}^{k_{\max}} \left(\frac{\tilde{U}_{ij;k}}{\tau^{2k}} x_s^{2k} + k \frac{H_{ij;0}}{\tau^{2k}} x_s^{2k} + (2k-1) \frac{Q_{ij;0}}{\tau^{2k-1}} x_s^{2k-2} \right.$$

$$\left. + 2 \frac{Q_{ij;0}}{\tau^{2k-1}} x_s^{2k-1} \frac{d}{dx_s} \right) \chi_{j;t}(x_s) = 0,$$

Unperturbed operator of 2D oscillator

For the OSQD (2D oscillator) with respect to the scaled slow **variable** x: $x_s = \rho = \sqrt{x/\sqrt{E_f})}$, where $E_f = (E_{i';0} + H_{i'i';0})/(4a^2) = \omega_{i'}^2/4$, i.e. adiabatic frequency, **at given** $i' = n_o$

$$L(n) = \mathrm{D}^{(0)} - E^{(0)}, \quad \mathrm{D}^{(0)} = -\left(\frac{d}{dx}x\frac{d}{dx} - \frac{x}{4} - \frac{m^2}{4x}\right),$$

$$E^{(0)} \equiv E^{(0)}_{n,m} = n + (|m| + 1)/2,$$

$$\Phi_q^{(0)}(x) = \frac{\sqrt{q!}x^{|m|/2}\exp(-x/2)L_q^{|m|}(x)}{\sqrt{(q + |m|)!}},$$

$$\int_0^\infty \Phi_q^{(0)}(x)\Phi_{q'}^{(0)}(x)dx = \delta_{qq'}.$$

Unperturbed operator of 2D oscillator

Therefore action of operators $L(n)$ and x **on function** $\Phi_q^{(0)}(x) \equiv \Phi_{q,m}^{(0)}(x)$ is determined by recurrence relations

$$
\begin{aligned}
& L(n)\Phi_{q,m}^{(0)}(x) = (q-n)\Phi_{q,m}^{(0)}(x), \\
& x\Phi_{q,m}^{(0)}(x) = -\sqrt{q+|m|}\sqrt{q}\Phi_{q-1,m}^{(0)}(x) + \\
& +(2q+|m|+1)\Phi_{q,m}^{(0)}(x) - \sqrt{q+|m|+1}\sqrt{q+1}\Phi_{q+1,m}^{(0)}(x), \\
& x\frac{d\Phi_{q,m}^{(0)}(x)}{dx} = -\sqrt{q+|m|}\sqrt{q}\Phi_{q-1,m}^{(0)}(x)/2 \\
& -\Phi_{q,m}^{(0)}(x)/2 + \sqrt{q+|m|+1}\sqrt{q+1}\Phi_{q+1,m}^{(0)}(x)/2.
\end{aligned}
$$

Expansion of solution by normalized basis functions

Eigenfunctions with respect to new scaled variable x are sought in the form of expansion by normalized basis functions $\Phi_q^{(0)}(x)$, $q = 0, 1, \ldots$. of the two or one dimensional oscillators with unknown coefficients $b_{j,s}$:

$$\chi_{j;t}(x) = \sum_{q=0}^{q_{\max}} b_{j,q;t}\Phi_q^{(0)}(x), \quad b_{j,q<0;t} = b_{j,q>q_{\max};t} = 0. \tag{1}$$

Substitution of expansion (1) leads to a set of equations

$$\sum_{q=0}^{q_{\max}} \hat{\mathbf{A}}_{ii} b_{i,q;t}\Phi_q^{(0)}(x) + \sum_{j\neq i=1}^{j_{\max}} \sum_{q=0}^{q_{\max}} \hat{\mathbf{A}}_{ij} b_{j,q;t}\Phi_q^{(0)}(x) = \sum_{q=0}^{q_{\max}} \kappa^{-2}\mathcal{E}_t E_f^{-1/2} b_{i,q;t}\Phi_q^{(0)}(x)$$

$$\hat{\mathbf{A}}_{ii} = \left(\mathrm{D}^{(0)} + \check{V}_s(x)E_f^{-3/4} + \kappa^{-2}E_{i;0}E_f^{-1/2} + \kappa^{-2}\sum_{k=1}^{k_{\max}} \frac{E_{i;0} + kH_{ii;0}}{\tau^{2k}E_f^{(k+1)/2}} x^{2k}\right)$$

$$\hat{\mathbf{A}}_{ij} = \kappa^{-2}\sum_{k=1}^{k_{\max}} \left(\frac{\tilde{U}_{ij;k} + kH_{ij;0}}{\tau^{2k}E_f^{(k+1)/2}} x_s^{2k} + \frac{Q_{ij;0}}{\tau^{2k-1}E_f^{k/2}}\left((2k-1)x^{2k-2} + 2x^{2k-1}\frac{d}{dx}\right)\right)$$

where $\kappa = 2$ and $\check{V}_s(x_s) = 0$ for OSQD and $\kappa = 1$ and $\check{V}_s(x) = \gamma_F x$ for PSQD.

Algebraic eigenvalue problem

Applying above recurrence relations for action of a first derivative on basis function, we get expressions for action of operators $\hat{\mathbf{A}}_{ij}$:

$$\hat{\mathbf{A}}_{ij}\Phi_q^{(0)}(x) = \sum_{q'=0}^{q_{\max}} \alpha_{ij;qq'}\Phi_{q'}^{(0)}(x)$$

and therefore, algebraic eigenvalue problem with respect to unknowns E_t and $b_{j,q;t}$

$$\sum_{q=0}^{q_{\max}} \alpha_{ii;q'q} b_{i,q;t} + \sum_{j\neq i=1}^{j_{\max}} \sum_{q=0}^{q_{\max}} \alpha_{ij;q'q} b_{j,q;t} = \kappa^{-2}\mathcal{E}_t E_f^{-1/2} b_{i,q;t}.$$

Algebraic eigenvalue problem

In matrix form it reads as

$$\mathbf{A}\mathbf{B}_t = \kappa^{-2}\mathcal{E}_t E_f^{-1/2}\mathbf{B}_t, \quad \mathbf{B}_{t'}^T\mathbf{B}_t = \delta_{tt'},$$

where $\mathbf{B}_t = (b_{1,0;t}, b_{1,1;t}, \ldots, b_{1,q_{\max};t}, b_{2,0;t}, \ldots, b_{j_{\max},q_{\max};t})^T$ is vector with dimension of $j_{\max}(q_{\max}+1)$ and $\mathbf{A}$ is positive defined symmetric matrix with dimension of $(j_{\max}(q_{\max}+1)) \times (j_{\max}(q_{\max}+1))$ with elements $A_{(q_{\max}+1)(i-1)+q+1,(q_{\max}+1)(j-1)+q'+1} = \alpha_{ij;qq'}$.

Result

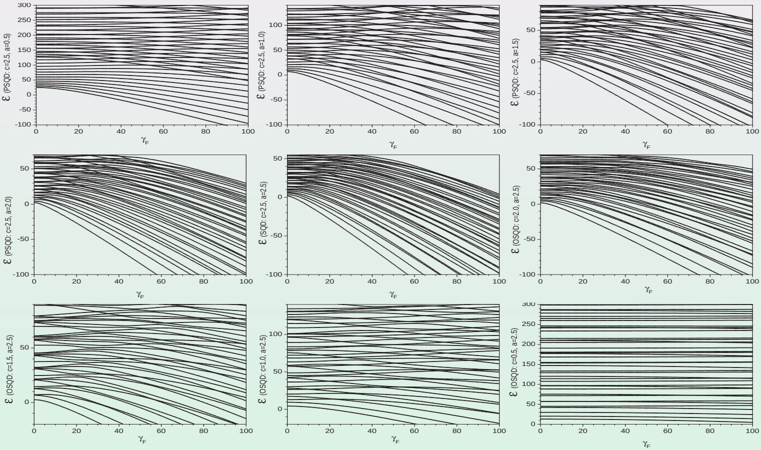
The convergence of eigenenergies $\mathcal{E}_t$ of Eq. (2) vs order $k_{\max}$ of approximation of effective potentials from (1) for $j_{\max} = 4$ and $q_{\max} = 60$ basis functions at $\gamma_F = 0$. Fast and slow variables $x_f = \rho$ and $x_s = z$ (*prolate* SQD and spherical QD), number of nodes $i = (n_{\rho p}, n_{zp})$.

$k_{\max}$	$c = 2.5,\ a = 0.5$			$c = 2.5,\ a = 2.5$		
i	(0,0)	(0,2)	(1,0)	(0,0)	(0,2)	(1,0)
8	25.179 14	34.076 77	126.445 9	1.471 911	4.270 174	5.614 892
12	25.199 62	34.468 84	126.456 0	1.536 121	4.716 984	6.188 144
20	25.201 16	34.522 02	126.456 1	1.563 492	5.182 198	6.266 533
N(4)	25.201 21	34.525 12	126.456 1	1.579 239	5.316 732	6.317 058

The same at $\gamma_F = -10$.

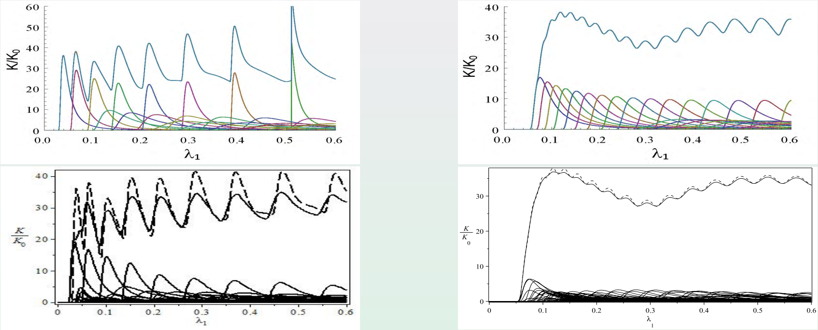
$k_{\max}$	$c = 2.5,\ a = 0.5,\ \gamma_F = -10$			$c = 2.5,\ a = 2.5,\ \gamma_F = -10$		
i	(0,0)	(0,2)	(1,0)	(0,0)	(0,2)	(1,0)
8	20.221 65	30.913 36	125.306 2	-19.673 98	-5.378 707	-1.784 110
12	20.607 33	32.375 40	125.331 6	-15.348 50	-6.881 266	-2.605 091
20	20.658 46	32.674 45	125.332 2	-12.194 45	-2.204 160	-1.336 853
N(4)	20.66203	32.708 77	125.332 2	-10.844 02	-1.511 063	1.129 039

Spectrum of electronic states of QDs vs electric field



Dependence of eigenenergies $\boldsymbol{\mathcal{E}}$ (in units of $\boldsymbol{E_e}$) of lower part of spectrum of electronic states of QDs at $\boldsymbol{m=0}$ on electric field strength $\boldsymbol{\gamma_F}$ (in units of $\boldsymbol{F_0^*}$): for spherical quantum dot (SQD) with radius $\boldsymbol{a=c=2.5}$, oblate and prolate spheroidal quantum dots (OSQD and PSQD) at different minor semiaxis (for OSQD $\boldsymbol{c=0.5,1,1.5,2}$, $\boldsymbol{a=2.5}$, for PSQD $\boldsymbol{c=2.5}$, $\boldsymbol{a=0.5,1,1.5,2}$).

Absorption coefficient of inter-band transitions in QDs



Absorption coefficient K/K_0 consists of sum of the first partial contributions vs the energy $\lambda = \lambda_1$ of the optic interband transitions for the Lifshits-Slezov distribution by using functions $f^{h-e}_{\nu,\nu'}(u)$ for GaAs $(h \longrightarrow e)$: (left panels) for assemble of OSQDs $\bar{c} = 0.5$, $a = 2.5$; (right panels) for assemble of PSQDs $\bar{a} = 0.5$, $c = 2.5$ in presence of electric field $\gamma_F = 10$ and $\gamma_F = 1$ (solid lines on lower panels) and without electric field $\gamma_F = 0$ (Upper panels and dashed line on lower panels).

Conclusion

•Symbolic-numerical algorithms for solving the BVPs are developed and elaborated in a problem-oriented complex of programs, now available via the Computer Physics Communication Library.

• The revealed difference in the spectra and the absorption coefficients allows verification of OSQD and PSQD models using the experimental data, e.g., photo-absorption coefficient and conductivity, from which not only the energy level spacing, but also the mean geometric dimensions of QDs can be estimated.

• The adiabatic approximations implemented in the both numerical and analytic forms can be applied also to treat a lower part of spectra of models of deformed nuclei.

• The results are also important for the experimental study of low-energy nuclear reactions of channeling ions in thin films and crystals by using elaborated Symbolic-Numerical Algorithms and Programs.