

# On the stationary Schrödinger equation describing electronic states of quantum dots in a magnetic field

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Semiconductor nanostructures have attracted tremendous interest in the past few years because of their special physical properties and their potential for applications in micro– and optoelectronic devices.

In such nanostructures, the free carriers are confined to a small region of space by potential barriers, and if the size of this region is less than the electron wavelength, the electronic states become quantized at discrete energy levels.

The ultimate limit of low dimensional structures is the quantum dot, in which the carriers are confined in all three directions, thus reducing the degrees of freedom to zero.

In this talk we consider the Zeeman splitting of energy levels of quantum dots (and rings) in a homogeneous magnetic field.

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# Problem

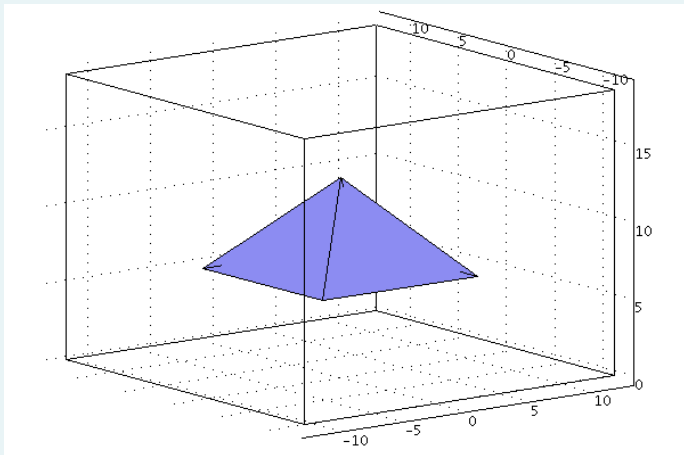


Figure: Pyramidal quantum dot embedded in a cuboid matrix

$$H = (-i\nabla + e\mathbf{A}) \frac{\hbar^2}{2m(\lambda, \mathbf{x})} (-i\nabla + e\mathbf{A}) + V(\mathbf{x}) + \mu_B \frac{g(\lambda, \mathbf{x})}{2} \boldsymbol{\sigma} \cdot \mathbf{B}$$

where

- $\hbar$  is the reduced Planck constant,
- $\nabla$  denotes the spatial gradient
- $\mathbf{A}(\mathbf{x})$  the vector potential such that  $\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{x})$  is the magnetic field intensity
- $m_0$  is the free electron mass,
- $\mu_B = \frac{e\hbar}{2m_0}$  is the Bohr magneton
- $\boldsymbol{\sigma}$  is the vector of Pauli matrices.

# Electron effective mass

The dependence of  $m(x, \lambda)$  on  $\lambda$  can be derived from the eight-band  $k \cdot p$  analysis and effective mass theory. Projecting the  $8 \times 8$  Hamiltonian onto the conduction band results in the single Hamiltonian eigenvalue problem with

$$m(x, \lambda) = \begin{cases} m_q(\lambda), & x \in \Omega_q \\ m_m(\lambda), & x \in \Omega_m \end{cases}$$

$$\frac{1}{m_j(\lambda)} = \frac{P_j^2}{\hbar^2} \left( \frac{2}{\lambda + E_{g,j} - V_j} + \frac{1}{\lambda + E_{g,j} - V_j + \Delta_j} \right), \quad j \in \{m, q\}$$

where  $m_j$  is the electron effective mass,  $V_j$  the confinement potential,  $P_j$  the momentum,  $g_j$  the main energy gap, and  $\Delta_j$  the spin-orbit splitting in the  $j$ th region.

The effective Landé factor  $g(\lambda, x)$  is given by

$$g_j(\lambda, x) := 2 \left\{ 1 - \frac{m_0}{m_j(\lambda)} \frac{\Delta_j}{3(\lambda + E_{g,j} - V_j) + 2\Delta_j} \right\}, \quad j \in \{m, q\},$$

where the material parameters are defined above.

Analogously to the effective mass, for a fixed energy level  $\lambda$ ,  $g(\lambda, x)$  is a piecewise constant function.

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# Schrödinger equation

The energy states and corresponding wave functions for electrons are obtained from the Schrödinger equation

$$\frac{1}{2m_j(\lambda)}(-i\hbar\nabla + e\mathbf{A}(x))^2\Phi + V_j\Phi + \mu_B\frac{g_j(\lambda)}{2}\sigma\mathbf{B}\Phi = \lambda\Phi, \quad j \in \{m, q\}, \quad (1)$$

and for physical applications the interesting eigenvalues are those in the interval  $(V_q, V_b)$ .

These eigenvalues are called confined states, since the corresponding wave functions  $\Phi$  live mainly on the quantum structure and decay rapidly outside of the structure. Hence, we may assume homogeneous Dirichlet conditions on the outer boundary of the matrix.

On the interface between the dot and the matrix the electron wave functions are continuous, and since  $A(x)$  is continuous the Ben Daniel–Duke condition is appropriate

$$\frac{1}{m_q(E)}\frac{\partial\Phi(x)}{\partial n_q} = \frac{1}{m_m(E)}\frac{\partial\Phi(x)}{\partial n_m}, \quad x \in \partial\Omega_{int},$$

where  $n_q, n_m$  denote the outward normal vector of the dot and the matrix.

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# Variational form of Schrödinger equation

Let  $\Omega := \overline{\Omega}_q \cup \Omega_m$ , and

$$H := \{ \phi : \Omega \rightarrow \mathbb{C} : \phi \in L^2(\Omega) \text{ and } (\nabla + i\mathbf{A})\phi \in L^2(\Omega), \phi = 0 \text{ on } \partial\Omega_{\text{out}} \}$$

with

$$\langle \phi, \psi \rangle := \int_{\Omega} (\nabla + i\mathbf{A})\phi \cdot \overline{(\nabla + i\mathbf{A})\psi} \, dx.$$

Find  $\lambda \in \mathcal{J} := (0, V_m)$  and  $\phi \in H$ ,  $\phi \neq 0$  such that

$$\begin{aligned} a_{\pm}(\phi, \psi; \lambda) &:= \frac{\hbar^2}{2m_q(\lambda)} \int_{\Omega_q} (\nabla + i\mathbf{A})\phi \cdot \overline{(\nabla + i\mathbf{A})\psi} \, dx \\ &+ \frac{\hbar^2}{2m_m(\lambda)} \int_{\Omega_m} (\nabla + i\mathbf{A})\phi \cdot \overline{(\nabla + i\mathbf{A})\psi} \, dx + V_m \int_{\Omega_m} \phi \bar{\psi} \, dx \\ &\pm \left( \gamma_q(\lambda) \int_{\Omega_q} \phi \bar{\psi} \, dx + \gamma_m(\lambda) \int_{\Omega_m} \phi \bar{\psi} \, dx \right) = \lambda \int_{\Omega} \phi \bar{\psi} \, dx =: \lambda b(\phi, \psi) \end{aligned}$$

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The following lemma contains a sufficient condition for  $a_{\pm}(\cdot, \cdot; \lambda)$  to be  $H$ -elliptic for all  $\lambda \in J$  such that each of the linear eigenvalue problems

Find  $\mu$  and  $\phi \in H$ ,  $\phi \neq 0$  with  $a_{\pm}(\phi, \psi; \lambda) = \mu b(\phi, \psi)$  for every  $\psi \in H$

has a countable set of eigenvalues  $0 < \mu_1^{\pm}(\lambda) \leq \mu_2^{\pm}(\lambda) \leq \dots$  which can be characterized by the minmax principle of Poincaré

$$\mu_j^{\pm}(\lambda) = \min_{\dim V=j} \max_{\phi \in V, \phi \neq 0} \frac{a_{\pm}(\phi, \phi, \lambda)}{b(\phi, \phi)}.$$

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## Lemma 1

Let  $\kappa_{\min}$  be the minimal eigenvalue of the linear eigenvalue problem

$$c(\phi, \psi) := \int_{\Omega} (\nabla + i\mathbf{A})\phi \cdot \overline{(\nabla + i\mathbf{A})\psi} \, dx = \kappa \int_{\Omega} \phi \bar{\psi} \, dx \quad \text{for every } \psi \in H.$$

If

$$\min \left\{ \frac{\hbar^2}{2m_q(\lambda)}, \frac{\hbar^2}{2m_m(\lambda)} \right\} > \frac{\max\{|\gamma_q(\lambda)|, |\gamma_m(\lambda)| - V_m\}}{\kappa_{\min}} \quad \text{for every } \lambda \in J,$$

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## Lemma 1

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# Existence of Rayleigh functional

## Lemma 2

Assume that the conditions of Lemma 1 hold, and

$$-\frac{\hbar^2}{2} \max \left\{ \left( \frac{1}{m_q(\lambda)} \right)', \left( \frac{1}{m_m(\lambda)} \right)' \right\} > \frac{\max\{|\gamma'_q(\lambda)|, |\gamma'_m(\lambda)|\} - 1}{\kappa_{\min}}$$

for every  $\lambda \in J$  where  $\kappa_{\min}$  is defined as before.

Then for every  $\phi \in H$ ,  $\phi \neq 0$  each of the real equations  $f_{\pm}$  satisfies

$$f_{\pm}(0; \phi) < 0 \quad \text{and} \quad \frac{\partial}{\partial \lambda} f_{\pm}(\lambda; \phi) > 0 \quad \text{for every } \lambda \in J.$$

Hence, equation

$$f_{\pm}(\lambda; \phi) := \lambda b(\phi, \phi) - a_{\pm}(\phi, \phi; \lambda) = 0$$

implicitly defines a Rayleigh functional  $p_{\pm} : H \supset D_{\pm} \rightarrow J$  for each of nonlinear Schrödinger eigenproblems where

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# Minmax Characterization

## Theorem

Assume that the conditions of Lemma 1 and Lemma 2 are satisfied. Then each of the Schrödinger equations has a finite number of eigenvalues in  $J$ , and it holds that

- (i) The  $k$ th smallest eigenvalue can be characterized by

$$\lambda_k^\pm = \min_{\dim V=k, V \cap D_\pm \neq \emptyset} \max_{\phi \in V \cap D_\pm} \rho_\pm(\phi).$$

- (ii) The minimum is attained for the subspace which is spanned by eigenfunctions corresponding to the  $k$  smallest eigenvalues of the linear eigenproblem

$$a_\pm(\phi, \psi, \lambda_k^\pm) = \mu b(\phi, \psi) \quad \text{for every } \psi \in H.$$

Equipped with this result we can devise efficient iterative projection methods, which compute approximations to the eigenvalues of the nonlinear problems safely one after another as it is done in the linear case.

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# Discretization

Discretizing the Schrödinger equation by a Rayleigh–Ritz method (finite elements, e.g.) one obtains a rational matrix eigenvalue problem

$$\begin{aligned} S_{\pm}(\lambda)x &:= \lambda Mx - \frac{\hbar^2}{2m_q(\lambda)} K_q x - \frac{\hbar^2}{2m_m(\lambda)} K_m x - V_m M_m x \\ &\pm (\gamma_q(\lambda) M_q + \gamma_m(\lambda) M_m) x = 0. \end{aligned}$$

and the involved matrices are given by

$$\begin{aligned} K_j^{(i,k)} &= \int_{\Omega_j} (\nabla + iA)\phi_i \overline{(\nabla + iA)\phi_k} dx \\ M^{(i,k)} &= \int_{\Omega} \phi_i \phi_k dx \\ M_j^{(i,k)} &= \int_{\Omega_j} \phi_i \phi_k dx. \end{aligned}$$

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# Nonlinear Arnoldi method

- 1: start with an initial pole  $\sigma$  and an initial orthonormal basis  $V$ ,  $V^T V = I$
- 2: determine preconditioner  $K \approx S(\sigma)$ ,  $\sigma$  close to the smallest eigenvalue
- 3:  $k=1$
- 4: **while**  $k \leq$  number of wanted eigenvalues **do**
- 5:   compute the  $k$ th smallest eigenvalue  $\mu$  and corresponding normalized eigenvector  $y$  of the projected problem  $V^T S(\mu) V y = 0$
- 6:   determine Ritz vector  $u = V y$  and residual  $r = S(\mu) u$
- 7:   **if**  $\|r\| < \varepsilon$  **then**
- 8:     accept eigenvalue  $\lambda_k = \mu$ , and eigenvector  $x_k = u$ ,
- 9:     choose new pole  $\sigma$  and update preconditioner  $K \approx S(\sigma)$  if indicated
- 10:    restart if necessary
- 11:     $k = k + 1$
- 12:    choose approximation to next eigenpair  $(\mu, u)$
- 13:    compute residual  $r = S(\mu) u$
- 14:    **end if**
- 15:    solve  $K v = r$  for  $v$
- 16:     $v = v - V V^T v$ ,  $\tilde{v} = v / \|v\|$ ,  $V = [V, \tilde{v}]$
- 17:    reorthogonalize if necessary
- 18: **end while**

A crucial point in iterative projection methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method from converging to the same eigenvalue repeatedly.

For linear eigenvalue problems this is easy to do by using Schur forms or generalized Schur forms for the projected problem and then locking or purging certain eigenvectors. For nonlinear problems, however, such normal forms do not exist and this presents one of the most difficult tasks in achieving good convergence.

For symmetric nonlinear eigenproblems satisfying a minmax characterization however, its eigenvalues can be computed safely one after the other: The minimum is attained for the invariant subspace of  $S(\lambda_k)$  corresponding to the  $k$  largest eigenvalues, and the maximum by every eigenvector corresponding to the eigenvalue 0.

This suggests the safeguarded iteration for computing the  $k$ th smallest eigenvalue for the projected eigenproblem  $P(\lambda)y := V^T S(\lambda) Vy = 0$ :

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This suggests the safeguarded iteration for computing the  $k$ th smallest eigenvalue for the projected eigenproblem  $P(\lambda)y := V^T S(\lambda) Vy = 0$ :

# Safeguarded iteration

- 1: Start with an approximation  $\mu_1$  to the  $k$ th smallest eigenvalue of  $P(\lambda)y = 0$
- 2: **for**  $\ell = 1, 2, \dots$  until convergence **do**
- 3:   determine an eigenvector  $u$  corresponding to the  $k$ th largest eigenvalue of the matrix  $P(\mu_\ell)$
- 4:   evaluate  $\mu_{\ell+1} = q_{\pm}(u)$ , i.e. solve  $u^T P(\mu_{\ell+1})u = 0$  for  $\mu_{\ell+1}$
- 5: **end for**

The safeguarded iteration has the following convergence properties (V., Werner (1984)):

- It converges globally to the smallest eigenvalue  $\lambda_1$ .
- The (local) convergence to simple eigenvalues is quadratic.
- If  $P'(\lambda)$  is positive definite, and  $u$  in Step 3 is replaced by an eigenvector of  $P(\mu_\ell)u = \mu P'(\mu_\ell)u$  corresponding to the  $k$ th largest eigenvalue, then the convergence is even cubic.
- Moreover, a variant exists which is globally convergent also for higher eigenvalues.

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# Numerical Example

Consider a pyramidal InAs quantum dot of height 6.2nm and width 12.4nm embedded into a cuboid GaAs matrix  $24.8 \times 24.8 \times 18.6 \text{ nm}^3$ , which we expose to a homogenous magnetic field perpendicular to the base of the pyramid of strengths 1, 5, 10, 15, 20, 25[T].

We discretized the pyramid and the matrix on a tetrahedral grid with quadratic Lagrangian elements.

The eigenfunctions decay rapidly outside of the dot and the coefficient functions of the differential operator have a jump on the interface. We therefore chose a nonuniform grid, which was fine on the interface between the dot and the matrix, coarser on the dot and coarse on the matrix.

We obtained a pair of rational matrix eigenvalue problems with 70276 degrees of freedom. For the magnetic fields under consideration the resulting matrix eigenvalue problems satisfy the conditions of the discrete versions of Lemmas 2 and 3, and therefore can be solved by the nonlinear Arnoldi method combined with safeguarded iteration.

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# Numerical Example

The physical background of the problem, i.e. the splitting of the electronic levels suggest that the eigenfunctions of the pair of problems have some common directions.

To verify our guess we perform the following experiment. We assemble eight eigenvectors  $X_-$  and  $X_+$  corresponding to the problem  $S_-$  and  $S_+$ , respectively, in one matrix and compute its singular value decomposition.

B	$\sigma_1$	$\sigma_2$	$\sigma_3$	$\sigma_4$	$\sigma_5$	$\sigma_6$	$\sigma_7$	$\sigma_8$	$\sigma_9$
5	1.618	1.553	1.422	1.414	1.407	1.340	1.261	1.194	0.0003
15	1.618	1.510	1.422	1.415	1.406	1.340	1.311	1.195	0.0008
25	1.618	1.485	1.423	1.416	1.404	1.395	1.340	1.197	0.0012

For all three values of  $B$  we observe a clear gap between the 8th and the 9th singular value whereas neither the singular values of  $X_+$  nor those of  $X_-$  contain an essential gap. This indicates that the eigensubspaces  $X_-$  and  $X_+$  overlap substantially. Though this effect wears off with growing  $B$  it is still of the order  $10^{-3}$  for a very large  $B = 25[T]$ .

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# Numerical Example

In view of this experiment it appears that solving the pair of problems  $S_{\pm}$  simultaneously allows the solution of one problem to benefit from the solution of the other. This leads to the following approach. We apply an iterative projection method to both problems simultaneously in such a way that they use the same search space  $\mathcal{V}$ .

There are many ways of combining the iterations. We just name the following three:

- 1 Fast alternating: We alternately expand the search space computing corresponding eigenpairs of  $S_+$  and  $S_-$  simultaneously.
- 2 Slow alternating: We alternately compute the wanted eigenpairs of  $S_-$  and  $S_+$  one by one;
- 3 Sequential: We compute all wanted eigenpairs of  $S_-$  first, then the wanted eigenpairs of  $S_+$ .

# Numerical Example

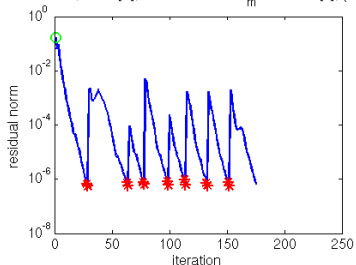
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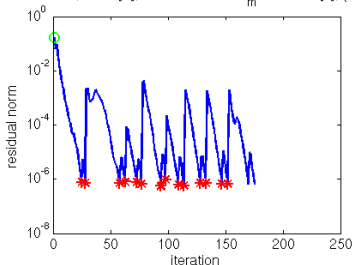
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# Convergence history, $B=5$ T

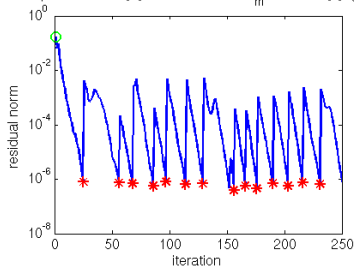
Fast alt.,  $B = 5$ [T], time for all  $\lambda < V_m = 243.79$  [s], (14)



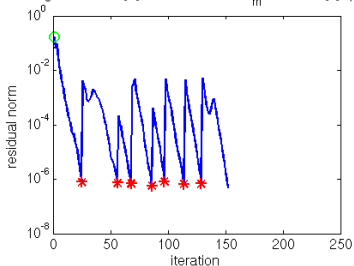
Slow alt.,  $B = 5$ [T], time for all  $\lambda < V_m = 241.94$  [s], (14)



Sequential,  $B = 5$ [T], time for all  $\lambda < V_m = 268.49$  [s], (14)

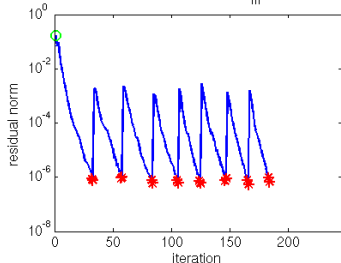


Negative,  $B = 5$ [T], time for all  $\lambda < V_m = 179.74$  [s], (7)

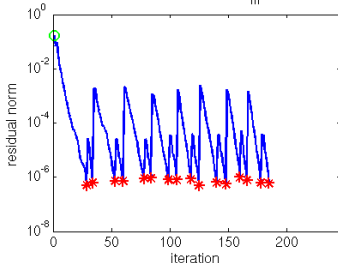


# Convergence history, $B=25$ T

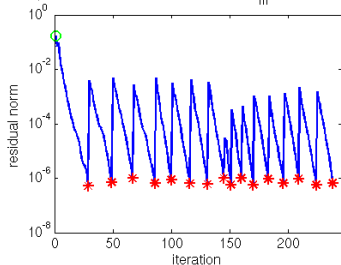
Fast alt.,  $B = 25$ [T], time for all  $\lambda < V_m = 363.07$  [s], (16)



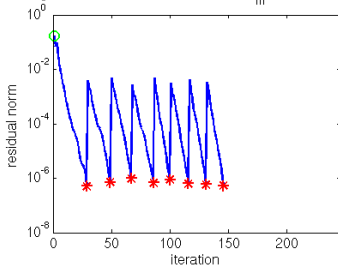
Slow alt.,  $B = 25$ [T], time for all  $\lambda < V_m = 367.06$  [s], (16)



Sequential,  $B = 25$ [T], time for all  $\lambda < V_m = 341.44$  [s], (16)



Negative,  $B = 25$ [T], time for all  $\lambda < V_m = 224.99$  [s], (8)



**Table:** Computation time for the Nonlinear Arnoldi method applied to compute 8 smallest eigenvalues of  $S_-$  and the slowly varying method applied to the pair  $S_{\pm}$ .

$B$	total time (N.Arn. $S_-$ ) [s]	#iter	total time (simultaneously) [s]	#iter
1	239.5	151	285.0	165
5	242.2	152	323.1	175
10	259.7	157	371.3	187
15	230.6	148	359.6	184
20	230.8	148	356.4	183
25	225.0	146	367.0	185

**Table:** Computation time for the Nonlinear Arnoldi method applied to  $S_-$  and the slowly varying method applied to the pair  $S_{\pm}$  for  $B = 25[T]$ .

$\pm$	$\lambda$	time (N.Arn.) [s]	time (simultaneously)
+	0.3673	-	26
-	0.3725	28.7	4.6
+	0.5131	-	19
-	0.5161	19.4	8.2
+	0.5565	-	23.3
-	0.5591	21	9
+	0.6380	-	24.5
-	0.6398	26.9	13.1
+	0.6480	-	24.4
-	0.6497	23.5	16.2
+	0.7352	-	37.7
-	0.7364	31	23.4
+	0.7488	-	38.1
-	0.7498	34.2	22
+	0.7613	-	46.2
-	0.7622	40.3	31.1

# Conclusions

We derived a pair of the nonlinear eigenvalue problems corresponding to the one–band effective Hamiltonian in magnetic field.

We derived conditions for the three dimensional problem to allow the minmax characterization of their relevant eigenvalues.

The problem requires numerical treatment with iterative projection methods as its discretization with Galerkin methods yields large and sparse rational matrix problems. Endowed with the minmax principle the method can effectively prevent the repeated convergence to the already computed eigenpairs.

We devised specially tailored methods simultaneously handling the pair of the problems and thereby saving about 25% in the three dimensional case of the overall computation time.

For rotationally symmetric problems (quantum rings in a magnetic field, e.g.) there is even a quadruple of Schrödinger equations which can be solved simultaneously thereby saving even up to 50% of the overall computing time.

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