A three-dimensional solver of the Schrödinger equation in momentum space for the detailed simulation of nanostructures

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Abstract

We propose a simple method for computing the single-particle eigenfunctions in nanostructures with three-dimensional confinement. The proposed procedure transfers the problem to the momentum space, solves an eigenvalue equation on a reduced wavevectors space and then transfers the solution back to the real space. We show that in such a way it is possible to obtain the eigenvectors and eigenvalues corresponding to lower energies with significant improvement in computing time and memory requirements with respect to numerical methods in the coordinate space. The method can be applied to structures with inhomogeneous effective mass and can easily include the full band structure. We have tested the code on typical confining potentials of nanostructures, in order to show the advantages and possible limitations of the proposed method.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Detailed simulation of nanoscale devices requires that quantum mechanical effects that emerge in the case of strong electron confinement be properly taken into account. The many-particle Schrödinger equation can usually be solved with density functional theory, and the local density approximation [1–3]. In such a framework, typical methods are based on the self-consistent solution of the nonlinear Poisson equation and of the single-particle Schrödinger equation.

In the case of three-dimensional confinement, the diagonalization of the Hamiltonian needed to solve the eigenvalue problem \( \hat{H}\Psi = E\Psi \) can require huge computational resources. Indeed, if we discretize the problem domain with a three-dimensional grid of \( N \times N \times N \) points we obtain a matrix of order \( N^3 \). In the case of the three-dimensional Schrödinger equation we obtain a symmetric matrix in which the non-zero elements are only in seven diagonals (7\( N \)). For large \( N \) the use of direct methods of diagonalization such as the Jacobi method or the Householder method [4] may become prohibitive. Since researchers are frequently interested only in eigenvalues and eigenvectors close to a particular energy level, selective methods that enable partial solutions of the eigenvalue problem have been successfully developed, such as, for example, those based on the method of powers or on the heat equation [4]. A commonly used technique consists in the so-called Lanczos methods, based on the tridiagonalization of the Hamiltonian, and in the direct solution of the tridiagonal matrix [5]. The possible convergence problems arising from the loss of orthogonality of the Lanczos vectors have been overcome by some authors with specific modifications of the standard algorithm [6]. Other authors have proposed selective relaxation methods characterized by strong stability in convergence [7], or the Hamiltonian variational approach [8].

We will show that transferring the eigenvalue problem to the momentum space provides significant advantages with respect to solving the problem in the coordinate space, in terms of computing time and memory requirements. In addition, it easily allows one to perform full band simulations, which is important in strongly confined structures, where the effective mass approximation may be inadequate.
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-1 that scale as 
the orthogonal basis \{v_n(x)\}. A natural choice for the basis functions would be the complex
functions \{e^{i k x}\} that imply the use of the fast Fourier
transform (FFT) algorithm. Nevertheless, in order to enforce
Dirichlet boundary conditions for the eigenfunctions, we use the
sine Fourier transform.
However, it is clear that, if the given function \( f(x) \) is quite
similar to the first vectors of the basis, it can be reasonably
approximated by a series truncated to lower order. In our code
we calculate the eigenfunctions by solving the Hamiltonian
in the \(-1\)-space and suppose that for a good approximation of
the first eigenfunctions it is sufficient to diagonalize a reduced
matrix, in which we retain only terms associated with smaller \( k \).
The advantage, from the point of view of memory requirements
(that scale as \( N \), where \( N \) is the matrix dimension) and of
computing time (that scales between \( N^2 \) and \( N^3 \)) is evident.

As an example, we first consider the eigenfunctions of
a triangular confining potential, for which we have the exact
analytical eigenfunctions. In figure 1 we plot the norm of
the error associated with the first low-energy eigenfunctions
obtained with different discretizations. With dotted curves we
indicate the errors due to a solution in the \(-1\)-space, versus
the number \( N \) of discretization points in the \(-1\)-space. Solutions
in the \(-1\)-space are obtained by first discretizing the equation
in the \(-1\)-space on 512 grid points, by transferring the problem
into the \(-1\)-space with the sine Fourier transform, by solving
the eigenvalue problem on a minor of dimension \( N \) of the
complete matrix, and finally by transferring back the solution to
the \(-1\)-space. The norm of the error associated with the solution
in the \(-1\)-space is plotted with solid curves as a function of \( N \). It
is worth noting that the computing time basically depends only

\[ \| \Psi_n - \Psi_0 \| \approx \begin{cases} \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial x} m^{-1}_n(x, y, z) + \frac{\partial}{\partial y} m^{-1}_n(x, y, z) \right] \Psi(x, y, z) & \text{in the } -1\text{-space (solid curves)} \\ \frac{1}{2} \left[ \mathcal{F}_c(V)(k_x - k'_x) - \mathcal{F}_c(V)(k_x + k'_x) \right] & \text{in the } -1\text{-space} \end{cases} \]

\[ \text{with obvious notation for the sine transform } \mathcal{F}_s \text{ and cosine transform } \mathcal{F}_c. \]

For example, the term relative to the sine Fourier transform
of \( \frac{\partial}{\partial x} m^{-1}_n(x, y, z) \Psi(x, y, z) \) is

\[ \int \int \int dk''_x dk'_x dk''_y \mathcal{F}_s(\Psi)(k''_x, k'_y, k''_y) \times \frac{\hbar^2}{4} \left[ \mathcal{F}_s(m^{-1}_n)(k_x - k'_x, k_y - k'_y, k_z - k'_z) - \mathcal{F}_c(m^{-1}_n)(k_x + k'_x, k_y + k'_y, k_z + k'_z) \right] 
- \mathcal{F}_c(m^{-1}_n)(k_x - k'_x, k_y - k'_y, k_z - k'_z) 
+ \mathcal{F}_c(m^{-1}_n)(k_x + k'_x, k_y + k'_y, k_z + k'_z) 
- \mathcal{F}_c(m^{-1}_n)(k_x - k'_x, k_y - k'_y, k_z - k'_z) 
+ \mathcal{F}_c(m^{-1}_n)(k_x + k'_x, k_y + k'_y, k_z + k'_z) \]

\[ \text{Figure 1. Two-norm of the difference between the analytic} \]
\[ \text{eigenfunctions } \Psi_0 \text{ (Airy functions) and those calculated from} \]
\[ \text{the diagonalization of the reduced Hamiltonian of order } N \text{ in the} \]
\[ \text{\(-1\)-space (solid curves)) and those obtained from the diagonalization} \]
\[ \text{of the Hamiltonian in the \(-1\)-space on } N \text{ grid points (dashed curves).} \]
\[ \text{The confining potential is a triangular well. Index } n \text{ indicates the} \]
\[ \text{\( n \)th eigenvector } (n = 1 \text{ is the lowest}). \]

\[ \text{on } N. \text{ It can been seen, for example, that if an error of } 10^{-4} \]
\[ \text{is required, we need to solve an eigenvalue problem of order} \]
\[ N = 512 \text{ in the coordinate space, and of only order } N = 32 \text{ in the} \]
\[ \text{\(-1\)-space. Since the computing timescale between } N^2 \text{ and} \]
\[ N^3, \text{ the time saving is a factor between } 64 \text{ and } 512. \]

\[ \text{The single-particle three-dimensional Schrödinger equation} \]
\[ \text{in the \(-1\)-space} \]
\[ \frac{-\hbar^2}{2} \left[ \frac{\partial}{\partial x} m^{-1}_n(x, y, z) + \frac{\partial}{\partial y} m^{-1}_n(x, y, z) \right] \Psi(x, y, z) \]
\[ + \frac{\partial}{\partial z} m^{-1}_n(x, y, z) \Psi(x, y, z) = E \Psi(x, y, z), \]
From figure 2 it can be noticed that the solution on a reduced exact analytic solution and the values obtained from an $k$-space reduces the eigenvalue problem by keeping only the matrix accuracy as a basis of 16 $k$-space or in the $k$-space provides the same accuracy as a basis of 16$^3$ elements in the $x$-space.

where

$$\mathcal{F}_s(f)(k_x, k_y, k_z) = \int \int \int dx \, dy \, dz \, \sin(k_x x) \, \sin(k_y y)$$

$$\times \sin(k_z z) \, f(x, y, z)$$

(3)

and

$$\mathcal{F}_c(f)(k_x, k_y, k_z) = \int \int \int dx \, dy \, dz \, \cos(k_x x) \, \cos(k_y y)$$

$$\times \cos(k_z z) \, f(x, y, z)$$

(4)

are, respectively, the sine transform and cosine transform of $f(x, y, z)$ and we have another similar expression for the other part of the Hamiltonian.

From the discretization of the three-dimensional generalization of equation (2) we find the matrix of the complete eigenvalue problem. Then we diagonalize only the sub-matrix corresponding to smaller $k$ vectors.

3. Simulations

In this section we show examples for evaluating the efficiency of the three-dimensional Schrödinger solver in the momentum space for typical confining potentials in nanostructures.

As a first test structure we consider a three-dimensional harmonic oscillator corresponding to different truncated bases in the $x$-space or in the $k$-space. A truncated basis of $8^3$ elements in the $k$-space provides the same accuracy as a basis of $16^3$ elements in the $x$-space.

Let us underline the fact that the main advantage comes from the fact that we can use a fine discretization in the $x$-space, in order not to lose the details of the confining potential, because the computational cost of performing an FFT of a matrix of order $16^3$ is negligible (smaller than 50 ms).

With the use of the proposed routine, the computing time for the solution of the single-particle Schrödinger equation becomes negligible with respect to the total time for the self-consistent solution of the Poisson–Schrödinger equation. Therefore, we can perform a complete diagonalization of the Hamiltonian with a simple well known code.

Footnotes:

1. Routines tred2 and tqli from [4].
2. See footnote 1.

Table 1. The CPU running time of an 800 MHz Pentium III required for the solution of the eigenvalue problem for a parabolic potential defined on a grid of $16 \times 16 \times 16$ points in the real space. The computing time for solving the problem in the $k$-space includes the FFT of the equation, the complete diagonalization and the anti-FFT of the eigenvectors.

<table>
<thead>
<tr>
<th>Sub matrix dimension</th>
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<tbody>
<tr>
<td>$16 \times 16 \times 16$ in the $k$-space</td>
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<tr>
<td>$16 \times 16 \times 16$ in the $x$-space</td>
<td>95 min (complete diag.)</td>
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<td>$16 \times 16 \times 16$ in the $x$-space</td>
<td>20 min (first ten eigenvalues)</td>
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Figure 2. The lowest 50 eigenvalues of a three-dimensional harmonic oscillator corresponding to different truncated bases in the $x$-space or in the $k$-space, compared with the analytic eigenvalues.

Figure 3. The lowest 50 eigenvalues of a cylindrical confining potential corresponding to different truncated bases in the $x$-space or the $k$-space. The cylinder has a circular basis with radius 10 nm and a height of 10 nm, and potential barriers of 1 eV.

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It is clear that the method takes advantage of the similarity between the sines of lower order and the eigenfunctions of the Hamiltonian related to smaller energies. Therefore, it provides the best performance in the case of strongly confined systems, where the confining region has a shape similar to the domain in which the Schrödinger equation is solved.

The second example we consider is a quantum dot defined by a cylindrical potential, with a circular base of radius 10 nm, a height of 10 nm and a confining energy of 1 eV. The data presented in figure 3 give the same results as figure 2, and shows that it is possible decrease the dimension of the Hamiltonian in the k-space to 8x8x8 points with the same accuracy of a solution on a 16x16x16 grid, while this would not be possible in the x-space. In this case, the potential in the x-space is discretized on a grid of 32^3 points.

As a third example we have simulated a lens-shaped quantum dot of InAs embedded in Al\sub{0.2}Ga\sub{0.8}As, with a radius of 10 nm and a height of 4 nm, shown in the inset of figure 4. The potential well has a height of 1.05 eV. The data presented in figure 4 gives the same results as the data presented in figures 2 and 3. Again, a solution on a basis of 8^3 elements in the k-space provides the same accuracy of a solution on 16^3 points in the coordinate space.

4. Conclusions
We have presented a method to solve the three-dimensional Schrödinger equation for systems with variable effective mass based on the expansion of the sine Fourier series. We have shown that this method allows us to solve the eigenvalue problem on a reduced matrix in the k-space, with negligible loss of accuracy, and significant saving in terms of computing time. This method also has the advantage of allowing full band simulations, which may be important for nanoscale structures when the parabolic approximation of the dispersion relation does not hold. We have shown that if we are interested only in the lower eigenvalues, the order of the matrix can be typically reduced by a factor 8, which typically means a corresponding reduction of the computing time by about two orders of magnitude. The same method is presently being applied to the solution of the Schrödinger equation with open boundary conditions.

Acknowledgment
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