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APPLICATION OF GRÖBNER BASIS IN CALCULATION OF WAVE FUNCTIONS IN NANOSTRUCTURES

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The knowledge of exact wave functions is required in calculating physical parameters such as optical dipole moments, scattering matrix elements, or in wave function engineering. In this report we describe how a system of algebraic equations that follows from the Schrödinger equation can be reduced to a Gröbner basis from which the exact wave function can be easily constructed. As an example, closed form solutions for a cylindrical electronic waveguide and double quantum well nanostructures are presented.

Keywords: Gröbner bases, semiconductor nanostructures, optical dipole matrix elements, wave function engineering

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1. Introduction

There is only a small number of quantum systems for which the exact wave functions are known. However, they play a crucial role in interpreting the quantum mechanics. The problem of finding a wave function can be solved numerically with powerful computers, however, a set of numbers in computer memory represents a particular case which may not always be true. In this report we shall demonstrate that the computer algebra may be useful in finding analytical solutions for complex wave functions which are not accessible by pen-and-paper methods. The key to the problem is the Gröbner basis [1, 2].

Roughly speaking, a Gröbner basis (GB) for a system of polynomial equations is a different system of simpler polynomials having the same roots as the original one [1, 2]. In paper [3] and handbook [4] various computer algorithms that exploit GB are summarized. The finding of the GB requires a lot of sorting work, therefore, as a rule, it is done by advanced computer algebra packages such as *Mathematica* or *Maple*. In this report we shall describe how the system of algebraic equations that follows from the Schrödinger equation can be reduced to GB and the exact wave functions extracted from therein. In Sec. 2 the Gröbner basis is explained for a novice in this field. In Sec. 3, as an example, closed form solutions for a cylindrical electronic waveguide and double quantum well nanostructure are presented.

2. The concept of GB

Many problems in physics lead to multivariate polynomial equations of type

$$\begin{aligned} &f_1(x_1, x_2, ..., x_n) = 0, \\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ &f_m(x_1, x_2, \ldots, x_n) = 0, \end{aligned} \tag{1}$$

where f_1, ..., f_m are polynomials in n unknowns x_i. The main task is to solve this system analytically. However, the solution is not always possible, or it may not exist at all. The GB algorithm tries either to

solve the polynomial system, or if the explicit solution is not possible to extract maximum of useful information about properties of the polynomial (1). The GB algorithm can be used to solve linear systems of equations as well, however, the strength of GB emerges in more difficult problems. The result is usually another system of simpler multivariate polynomials which has the same zeroes as the original one. For example, if the solved polynomial system, with $x_1 = x$ and $x_2 = y$, is

$$\begin{aligned} x^3 + yx^2 - y^2 &= 0, \\ 2xy^2 + x^2 - y + 1 &= 0, \end{aligned} \qquad (2)$$

then its GB found by *Mathematica* has the following form:

$$\begin{aligned} 1 - 3y + 4y^2 - 3y^3 - 2y^4 + 4y^5 - 4y^7 + 8y^8 &= 0, \\ x - 1 + y + y^2 + 2y^4 + 4y^5 &= 0. \end{aligned} \qquad (3)$$

The original (2) and GB (3) polynomials have the same roots. However, the GB representation has advantage that at least one of the polynomials has the leading terms as a pure power of sought variable. In our case this is the first polynomial of 8th power in variable y. From (3) it is clear that the initial polynomial (2) cannot be solved exactly. If we know one of the roots y_i, the second polynomial in (3) shows how another root x_i can be found. In manipulations with multivariate polynomials the ordering of individual polynomial terms is important, since when more than one variable is involved we need a rule to decide which of the terms in the polynomial is larger or smaller. This brings into play lexicographic, graded lexicographic or other orderings of the GB polynomials [1, 2] that can be used in finding the optimal solution.

As a second example let us consider the following parametric equation of variable t that describes the curve on x–y plane,

$$\begin{aligned} x &= t\,(t-1)\,(t-2), \\ y &= (t-1)\,(t-2)\,(t-3). \end{aligned} \qquad (4)$$

The aim is to eliminate the parameter t and find a polynomial equation $p(x, y) = 0$. The solution is straightforward if the lexicographical order is used and the parameter t is allowed to be the first in the *Mathematica* GB package, i. e. the order in the input should read $\{t, x, y\}$. The calculations give the following GB that consists of four GB basis equations:

$$\begin{aligned} -6x^2 + x^3 - 15xy - 3x^2y - 6y^2 + 3xy^2 - y^3 &= 0, \\ 6x - x^2 - 6y + 9ty + 2xy - y^2 &= 0, \\ -21x + 9tx - x^2 - 6y + 2xy - y^2 &= 0, \\ 6 - 9t + 3t^2 - x + y &= 0. \end{aligned} \qquad (5)$$

Only the first of equations in (5), which is independent of t, provides the required solution to the posed problem. This problem may be also looked upon as a projection of the spatial curve in variables $\{t, x, y\}$ onto x–y plane.

Below we shall demonstrate how to apply GB theory in solving a kind of a combination of the two above-discussed examples, where both the solution of polynomial system and projection onto a smaller subspace is required. In particular, we want to find the coefficients that characterise the wave function of the nanostructure and at the same time to eliminate the eigenenergies. The complication is that the eigenenergies are determined by a transcendental dispersion equation which cannot be solved explicitly.

3. Application of GB to nanostructures

Figure 1 shows possible profiles of cylindrical electronic guides that are important in semiconductor nanoelectronics. Below only a cylindrical double quantum well (CDQW) is considered. We shall demonstrate that with the help of GB algorithm it appears possible to find analytical closed form solutions for wave function in general case even when the potential energies and effective masses are different in all regions as shown in Fig. 1(d).

3.1. Cylindrical double quantum well

For cylindrical guides the total eigenfunction is a product of three functions:

$$\Psi_{lnk_z}(\rho, z, \varphi) = \psi_{lnk_z}(\rho)\mathrm{e}^{\mathrm{i}l\varphi}\mathrm{e}^{\mathrm{i}k_z z}/N_{lnk_z}. \qquad (6)$$

where k_z is the wave vector along cylinder axis, $l = 0, \pm 1, \pm 2, \ldots$ is the angular momentum quantum number, and $n = 0, 1, 2, \ldots$ is the quantum number that describes spatial quantization in the radial

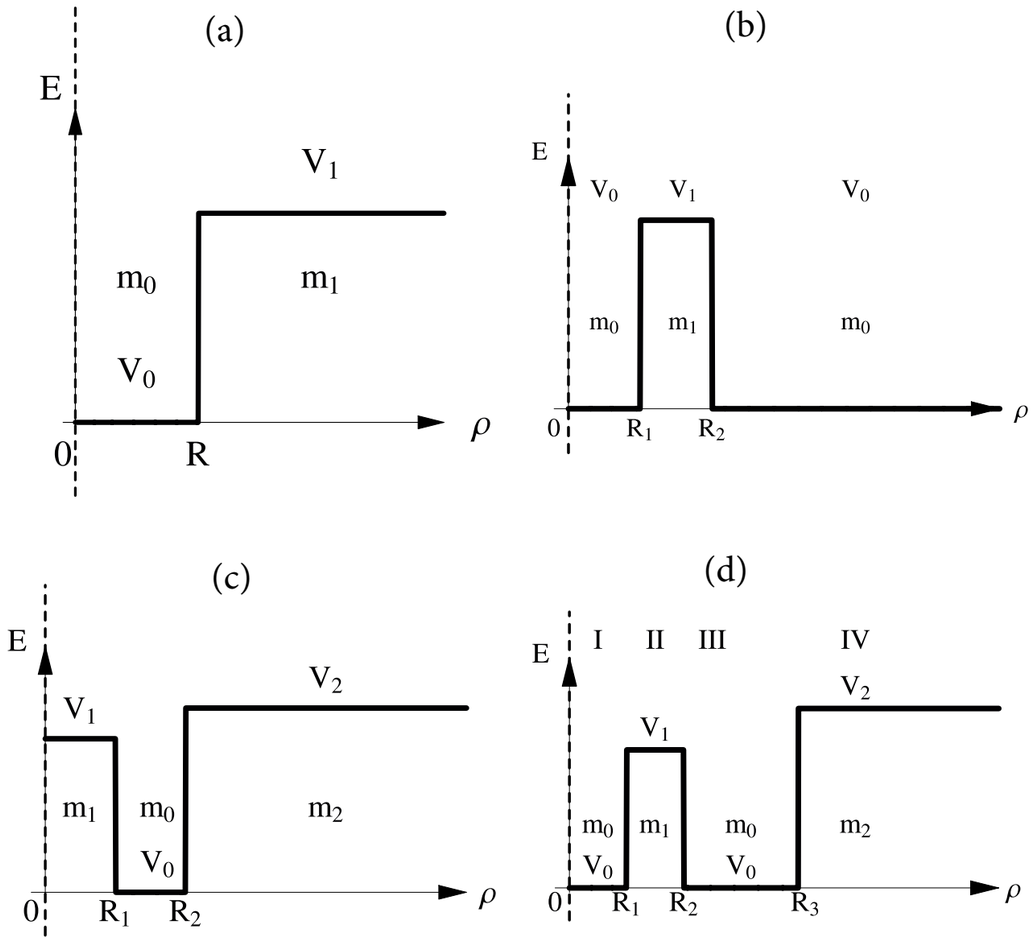

Fig. 1. Profiles of potential energy as a function of radius ρ for various semiconductor electronic guides having cylindrical symmetry: (a) simple guide, (b) higher-mode-stripper that supports only the lowest energy quasistationary modes with long tunneling lifetime, (c) tube-type, (d) cylindrical double quantum well (CDQW). Vertical dashed line indicates symmetry axis.

direction ρ. N_{lnk_z} is the normalization constant. The radial part $\psi_{lnk_z}(\rho) \equiv \psi$ satisfies equation ($\hbar = 1$)

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\rho^2} + \frac{m_\rho}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\frac{\rho}{m_\rho}\right)\frac{\mathrm{d}\psi}{\mathrm{d}\rho} + \left(K_\rho^2 - \frac{l^2}{\rho^2}\right)\psi = 0, \qquad (7)$$

where the wave vector K_ρ depends on kinetic E and potential V_ρ energies. In the following we shall limit ourselves to CDQW, Fig. 1(d), where regions I and III represent cylindrical wells. For CDQW having flat energy bands the potentials and electron effective masses in the wells are $V_\rho = V_0 = 0$, $m_\rho = m_0^*$, while in the barrier regions they are $V_\rho = V_i > 0$, $m_\rho = m_i^*$. Then the wave vector K_ρ becomes

$$K_0 = \sqrt{2m_0^* E - k_z^2}, \qquad (8)$$

$$K_i = \sqrt{2m_i^*(V_i - E) + k_z^2}\,. \tag{9}$$

The flat band assumption allows us to express solutions in different regions via Bessel functions. Below we shall demonstrate that this problem, which mathematically is rather complicated, is accessible analytically (at least eigenfunctions) if one resorts to computer based GB algorithm, which can be found in advanced computer algebra packages such as *Mathematica* or *Maple*. Since final expressions are long, the results will be presented in a graphical form. By the same reason it is recommended to do all related analytical calculations by computer[1].

We shall consider only the bound states of ψ when $E < V_1$, V_2. Then the wave function ψ for a piecewise flat potentials expressed through appropriate Bessel functions is, Fig. 1(d),

$$\psi = \begin{cases} \psi_{\rm I} = A_1 \mathrm{J}_n(k_1\rho) & \text{if } 0<\rho<R_1, \\ \psi_{\rm II} = B_1 \mathrm{K}_n(k_2\rho) + B_2 \mathrm{I}_n(k_2\rho) & \text{if } R_1<\rho<R_2, \\ \psi_{\rm III} = A_2 \mathrm{J}_n(k_1\rho) + A_3 \mathrm{Y}_n(k_1\rho) & \text{if } R_2<\rho<R_3, \\ \psi_{\rm IV} = B_3 \mathrm{K}_n(k_3\rho) & \text{if } \rho > R_3. \end{cases} \tag{10}$$

The unknown coefficients A_i and B_i are determined from the continuity of the total wave function and its derivatives at three interfaces with coordinates R_1, R_2 and R_3, Fig. 1(d). By integrating over vanishingly small cylindrical regions embracing respective interfaces it can be shown [5] that the boundary condition for derivatives is $m_{i+1}^* \psi_i'(\rho) = m_i^* \psi_{i+1}'(\rho)$ which coincides with that of BenDaniel–Duke boundary condition for a plane heterojunction [6].

The boundary conditions yield a system of linear homogeneous equations for coefficients A_i and B_i in equations (10),

$$\begin{aligned} &f_1(A_1, \ldots, B_3) = 0, \\ &\cdots\cdots\cdots\cdots\cdots \\ &f_6(A_1, \ldots, B_3) = 0. \end{aligned} \tag{11}$$

The determinant of (11) gives the transcendental equation for spectrum,

$$\mathrm{Det}\,[f_1, \ldots, f_6] = 0. \tag{12}$$

[1] The details of the calculation can be downloaded in a form of *Mathematica* notebook from http://mokslasplius.lt/files/DCQW.nb

Equation (12) is a sum of products of Bessel functions. The solution of (12) gives discrete energies that will be labelled by radial quantum number n = 0, 1, 2,..., which represents spatial quantisation of the wave function in ρ direction. Thus, in general the allowed energies E_{lnk_z} are characterised by three quantum numbers.

The next step is to calculate the coefficients A_i and B_i that satisfy the eigenvalue equation (12) with eigenfunctions ψ_{lnk_z}. This can be done analytically without solving the transcendental equation (12) if computer based GB algorithm is used. ψ_{lnk_z} calculated in this way depends on wave vectors K_0 and K_i given by (8) and (9) rather than on the eigenvalues E_{lnk_z}. However, to get nonzero coefficients the system (11) must be supplemented by the transcendental equation (12). This is important. If GB is applied to the system (11) only, then the trivial result $A_1 = \ldots = B_3 = 0$ is obtained. Some technical notes in finding the GB are appropriate here:

1. During calculation (this takes about three hours) of the GB the *Mathematica* program tries to simplify those expressions where complex combinations of Bessel functions appear. As a result, the program spoils the GB algorithm. To prevent this, one should rename the Bessel functions by some neutral symbols. Also, with the help of recursion relations the Bessel functions of same kind should be reduced to two adjacent ones, say, n and $n + 1$.
2. In the case of an open cylindrical quantum well, Fig. 1(b), where the electron is in the quasistationary state, the Breit–Wigner S-matrix method to evaluate lifetime of the states may be used if wave vectors are complex-valued [7].
3. The GB allows one to find five of the coefficients in ψ, Eq. (10). The last one, for example, B_3, should be calculated from the normalisation condition. This coefficient appears the most complex, however, frequently the normalisation of the functions not required.
4. Due to symmetry in $\pm z$ directions, the spectrum in the vicinity of the point $k_z = 0$ should be parabolic, $E_{lnk_z} = \hbar^2 k_z^2 / 2m_{k_z}^*$. The effective mass $m_{k_z}^*$ in principle can be calculated if the wave function with discrete quantum numbers l and n is known.

Figure 2 illustrates the wave functions of different modes calculated analytically for parameter values of compound semiconductor

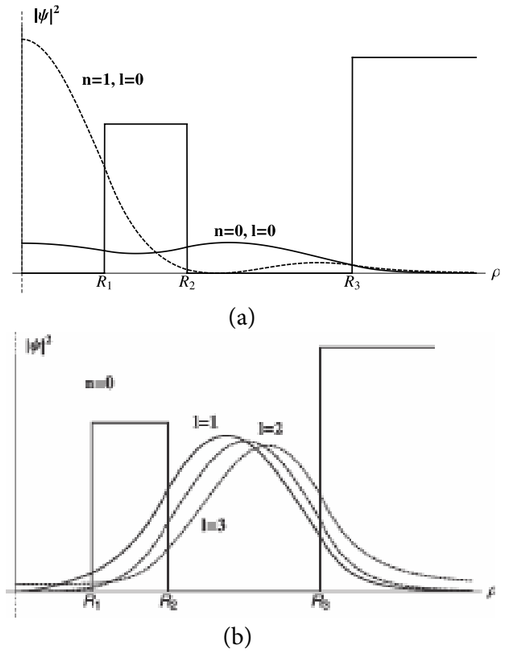

Fig. 2. Radial part of the wave function calculated analytically at following radial n and angular l quantum numbers: (a) n = 0, 1 and l=0; (b) n = 0 and l = 1, 2, 3. In all cases k_z = 0. The straight lines show potential profile in CDQW in radial direction.

$Ga_{1-x}As/Ga_{1-x}Al_xAs$ with V_0 = 0, V_1 = 177 meV, V_2 = 256 meV and respective masses $m_0^* = 0.067\,m_e$, $m_1^* = 0.0863\,m_e$, $m_2^* = 0.0919\,m_e$, where m_e is the electron mass in vacuum. It was assumed that radii in Fig. 1(d) are R_1 = 2 nm, R_2 = 4 nm, R_3 = 8 nm. Under these parameter values and at k_z = 0, we find that only five discrete energy levels E_{ln} can be supported by CDQW. At zero angular momentum, l = 0, the respective energies are E_{00} = 78.4527 meV, E_{01} = 201.86 meV. Figure 2(a) shows that the ground level wave function is relatively flat, while the first excited one is more concentrated in the centre of the CDQW. When $l \neq 0$ and n = 0 we find that E_{10} = 106.877 meV, E_{20} = 159.089 meV, E_{30} = 230.459 meV, and as can be seen from Fig. 2(b) the respective wave functions are shifted off the centre of CDQW. The larger quantum number l is, the larger shift is observed due to a larger effective centrifugal force.

3.2. Square double quantum well

Similar calculations have been performed for a square double quantum well, where instead of Bessel functions, trigonometric and hyperbolic functions appear. Figure 3 demonstrates the electrical dipole moment between the lowest energy levels. In calculating the dipole moment integrals one has to use explicit expressions for wave functions. The GB algorithm allows one to find such wave functions in a closed analytical form without solving the transcendental equation for spectrum as well as eigenvector equation. For further details the reader should refer to the paper [8].

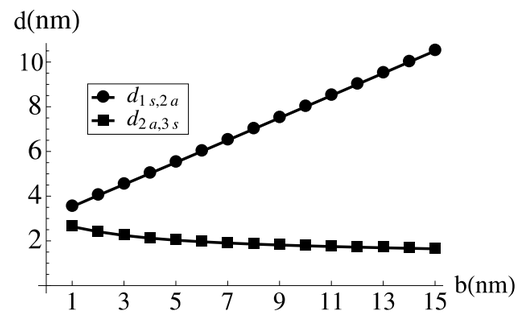

Fig. 3. Dipole matrix elements $d_{1s,\,2a}$ and $d_{2a,\,3s}$ (s and a indicates symmetric and antisymmetric wave functions, the numbers 1, 2 and 3 are the lowest energy levels) as a function of inner barrier width b for plane double quantum well calculated with the GB algorithm.

In conclusion, with the help of the Gröbner basis and computer algebra we have been able to find analytical expressions for wave functions of rather complicated quantum systems which normally are accessible by numerical methods only. This opens new perspectives in quantum wave function engineering.

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GROEBNERIO BAZĖS TAIKYMAS NANODARINIŲ BANGINIŲ FUNKCIJŲ SKAIČIAVIMUOSE

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Santrauka

Skaičiuojant fizikinius parametrus, tokius kaip optinius dipolinius momentus, kvantinių šuolių matricinius elementus, o bendresniu atveju dirbant kvantinėje inžinerijoje, būtina žinoti tikslias kvantines bangines funkcijas. Straipsnyje aprašyta, kaip galima redukuoti algebrinių lygčių sistemą, kuri išeina iš Schroedingerio lygties į Groebnerio bazę, o iš pastarosios sukonstruoti tikslias bangines funkcijas. Kaip metodo taikymo pavyzdys, straipsnyje suskaičiuotos elektrono pagrindinio ir sužadintų lygmenų banginės funkcijos cilindriniame bangolaidyje ir dvigubame kvantiniame šulinyje.