SPIN – A Schrödinger Poisson Solver Including Non-parabolic Bands

H. Kosina and C. Troger
Institute for Microelectronics, TU-Vienna, Gusshausstrasse 27-29, A-1040 Vienna, Austria
Phone +43/1/58801-3719, FAX +43/1/5059224, e-mail kosina@iue.tuwien.ac.at

A self-consistent Schrödinger Poisson solver has been developed capable of computing the subband structure of a quasi-two dimensional electron gas formed in silicon inversion layers or in various heterostructures. The employed model features position-dependent material parameters and a non-parabolic band structure.

In bulk semiconductors one frequently introduces non-parabolicity by using an E–$\vec{k}$ dispersion relation of the form $E(1+\alpha E) = \hbar^2\vec{k}^2/2m^*$, which results from the two-band Kane Model (see e.g. [1]). Such a model is expected to be accurate enough in many cases of interest and, in any case, can be used to to draw qualitative conclusions about non-parabolicity effects [2]. Assuming quantization in one dimension we replace the scalar quantities z and k_z by the operators $\mathbf{z}$ and $\mathbf{k}_z$, respectively, and end up with the following implicit definition of the kinetic energy operator $\mathbf{T}$:

$$\mathbf{T} + \mathbf{T}\,\alpha(\mathbf{z})\,\mathbf{T} = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x(\mathbf{z})} + \frac{k_y^2}{m_y(\mathbf{z})} + \mathbf{k}_z\frac{1}{m_z(\mathbf{z})}\mathbf{k}_z\right) \tag{1}$$

The in-plane wave vector is represented by $\vec{K} = (k_x, k_y)$. Expression (1) accounts for spatially varying material parameters such that multi-layer structures can be treated properly. The one-dimensional Schrödinger equation including the kinetic energy operator defined by (1) is solved numerically. As base functions we use the eigen functions of the momentum operator, $\hbar\mathbf{k}_z$, i.e., the wave functions are represented as Fourier series, and the unknowns of the equation system are the Fourier coefficients. On the other hand, to solve Poisson's equation finite difference discretization in real-space is used in order to take advantage of the sparsity of the equation system. The repeatedly required conversions from momentum to real-space representation and vice versa are accomplished by means of the fast Fourier transform (FFT).

Each subband can be characterized by an effective mass, m_n, and a non-parabolicity factor, α_n, two parameters which are extracted by applying perturbation theory at $\vec{K} = \vec{0}$. To describe the in-plane dispersion relation it appears favorable to use again an expression of the form $\epsilon_n(1+\alpha_n\epsilon_n) = \hbar^2\vec{K}^2/2m_n$. One consequence of non-parabolicity is that the wave functions depend on the in-pane wave vector. Their effective widths decrease with with higher in-plane momentum.

Acknowledgement This work has been supported by the *"Fonds zur Förderung der wissenschaftlichen Forschung"*, Project No. P10642 PHY.

[1] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Les Ulis, Cedex, France, 1992).

[2] J. López-Villanueva, I. Melchor, P. Cartujo, and J. Carceller, Physical Review B **48**, 1626 (1993).