9:40am T38 A Consistent Inclusion of Nonparabolicity in a Schrödinger-Poisson Solver for Silicon Inversion Layers

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We present a formalism for the consistent inclusion of nonparabolicity in the description of a quasi two-dimensional electron gas in silicon inversion layers.

For the characterization of the confined electrons the eigenenergies and wave functions are obtained from a self-consistent solution of the one-dimensional Schrödinger and Poisson equation. Starting from the well known nonparabolic $E - \mathbf{k}$ dispersion relation used for bulk semiconductors, we employ the momentum representation and use second order perturbation theory to solve the eigenvalue problem and to define an effective mass and a nonparabolicity coefficient in each subband. By restricting the dimension of the base to some final value all quantum mechanical operators are expressed as matrices. The extracted parameters and the eigenenergies are used in the Schroedinger-Poisson solver for the self-consistent iterations; their final values form a base set for the calculation of scattering rates needed in a subsequent multisubband Monte Carlo simulation. With our model we avoid the numerical drawbacks arising from the truncation of a polynomial approximation.

Using this formalism we have studied the influence of the in-plane wave vector on the wave functions and the variation of the in-plane dispersion relation in different subbands. As the treatment of more than 20 subbands can be performed in a realistic time, the formalism yields parameters needed for high-field electron transport calculations.