A Hybrid Method for Computing the Schrödinger Equations with Periodic Potential with Band-Crossings in the Momentum Space

Lihui Chai\textsuperscript{1}, Shi Jin\textsuperscript{2,*} and Peter A. Markowich\textsuperscript{3}

\textsuperscript{1}Department of Mathematics, University of California, Santa Barbara, USA.
\textsuperscript{2}Department of Mathematics, University of Wisconsin-Madison, Madison, WI 53706, USA, and Institute of Natural Sciences, School of Mathematical Science, MOE-LSEC and SHL-MAC, Shanghai JiaoTong University, Shanghai 200240, China.
\textsuperscript{3}Applied Mathematics, Computer Sciences and Electrical Engineering Division, KAUST (King Abdullah University of Science and Technology), Thuwal 23955-6900, Kingdom of Saudi Arabia.

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Abstract. We propose a hybrid method which combines the Bloch decomposition-based time splitting (BDTS) method and the Gaussian beam method to simulate the Schrödinger equation with periodic potentials in the case of band-crossings. With the help of the Bloch transformation, we develop a Bloch decomposition-based Gaussian beam (BDGB) approximation in the momentum space to solve the Schrödinger equation. Around the band-crossing a BDTS method is used to capture the inter-band transitions, and away from the crossing, a BDGB method is applied in order to improve the efficiency. Numerical results show that this method can capture the inter-band transitions accurately with a computational cost much lower than the direct solver. We also compare the Schrödinger equation with its Dirac approximation, and numerically show that, as the rescaled Planck number $\varepsilon \to 0$, the Schrödinger equation converges to the Dirac equations when the external potential is zero or small, but for general external potentials there is an $O(1)$ difference in between the solutions of the Schrödinger equation and its Dirac approximation.

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Key words: Schrödinger equation, band-crossing, Dirac point, Bloch decomposition, time-splitting spectral method, Gaussian beam method.

*Corresponding author. Email addresses: chai@ucsb.edu (L. Chai), sjin@wisc.edu (S. Jin), peter.markowich@kaust.edu.sa (P. A. Markowich)
1 Introduction: The Schrödinger equation with periodic potential

The linear Schrödinger equation with periodic potentials is an important model in solid state physics. It describes the motion of electrons in a crystal with a lattice structure. We consider the following Schrödinger equation in the semiclassical scaling

$$i \varepsilon \partial_t \psi_\varepsilon(t,r) = -\frac{\varepsilon^2}{2} \Delta_r \psi_\varepsilon(t,r) + \left( V_T(\frac{r}{\varepsilon}) + U(r) \right) \psi_\varepsilon(t,r), \quad r \in \mathbb{R}^d, \quad t \in \mathbb{R},$$

where $\psi_\varepsilon$ is the complex-valued wave function, $0 < \varepsilon \ll 1$ is the dimensionless rescaled Planck constant, $U = U(x)$ is a smooth real-valued external potential function, and $V_T$ is a (real) periodic potential function with linearly independent lattice vectors $\{v_1, v_2, \ldots, v_d\}$ of $\mathbb{R}^d$, i.e.

$$V_T(r + v) = V_T(r) \quad \text{for all} \quad v = \sum_{j=1}^d m_j v_j, \quad m_j \in \mathbb{Z}. \quad (1.2)$$

The lattice is then denoted by

$$\Gamma = \left\{ \sum_{j=1}^d m_j v_j, m_j \in \mathbb{Z} \right\}, \quad (1.3)$$

and the fundamental domain of the lattice $\Gamma$ is $C = \left\{ \sum_{j=1}^d x_j v_j, x_j \in [0,1] \right\}$. The reciprocal lattice $\Gamma^*$ is generated by the vectors $k_j$ for $1 \leq j \leq d$ which are defined by $v_j \cdot k_j = \frac{2\pi}{\varepsilon} \delta_{ij}$, where we denote the Kronecker delta by $\delta_{ij}$. Then the first Brillouin zone is given by $B = \left\{ \sum_{j=1}^d \xi_j k_j, \xi_j \in [-1/2,1/2] \right\}$.

The asymptotic behavior of the solution $\psi_\varepsilon$ of (1.1) as $\varepsilon \to 0$ has been intensively studied. One of the most striking effects is that the electrons remain semiclassically in a certain quantum subsystem, “move along the $m$-th band” and the dynamics is given by

$$\dot{r} = \partial_r E_m(k), \quad \dot{k} = -\partial_k U, \quad \text{where} \quad E_m \quad \text{is the energy corresponding to the $m$-th Bloch band} \quad [9],\quad \text{and} \quad U \quad \text{is the external potential. This result has been justified both from a physical point of view in, e.g. \cite{4, 42}, and from a mathematical point of view in, e.g. \cite{6, 7, 18, 30}. Higher order corrections relevant to the Berry phase can be included, see e.g. \cite{15, 34, 35}. One remark is that all of these results use the adiabatic assumption, namely different Bloch bands are well-separated and there is no band-crossing. Nevertheless the inter-band transition effect should be considered whenever the transitions between energy bands of the quantum system play an important role. This may happen when the gap between the energy bands becomes small enough in comparison to the scaled Planck constant $\varepsilon$ or at conical crossings where the bands intersect. The study of such “quantum tunnelings” is important in many applications, from quantum dynamics in chemical reaction \cite{39}, semiconductors to Bose-Einstein condensation \cite{10}. Mathematical studies on band-crossings can be found in e.g. \cite{20, 26, 29}. One of the most interesting applications of (1.1) is when $\Gamma$ has