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

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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 $\mathcal{O}(1)$ difference in between the solutions of the Schrödinger equation and its Dirac approximation.

AMS subject classifications: 35Q41, 65M70, 81Q20, 74Q10, 35B27

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

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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

$$\mathrm{i}\varepsilon\partial_t\psi^\varepsilon(t,\boldsymbol{r}) = -\frac{\varepsilon^2}{2}\Delta_{\boldsymbol{r}}\psi^\varepsilon(t,\boldsymbol{r}) + \left(V_\Gamma\left(\frac{\boldsymbol{r}}{\varepsilon}\right) + U(\boldsymbol{r})\right)\psi^\varepsilon(t,\boldsymbol{r}), \quad \boldsymbol{r}\in\mathbb{R}^d, \quad t\in\mathbb{R}, \tag{1.1}$$

where ψ^ε 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_Γ is a (real) periodic potential function with linearly independent lattice vectors $\{\boldsymbol{v}_1,\boldsymbol{v}_2,\cdots,\boldsymbol{v}_d\}$ of $\mathbb{R}^d$, *i.e.*

$$V_\Gamma(\boldsymbol{r}+\boldsymbol{v}) = V_\Gamma(\boldsymbol{r}) \quad \text{for all} \quad \boldsymbol{v} = \sum_{j=1}^d m_j\boldsymbol{v}_j, \ m_j\in\mathbb{Z}. \tag{1.2}$$

The lattice is then denoted by

$$\Gamma = \left\{\sum_{j=1}^d m_j\boldsymbol{v}_j, m_j\in\mathbb{Z}\right\}, \tag{1.3}$$

and the fundamental domain of the lattice Γ is $\mathcal{C}=\left\{\sum_{j=1}^d x_j\boldsymbol{v}_j, x_j\in[0,1]\right\}$. The reciprocal lattice Γ^* is generated by the vectors $\boldsymbol{k}_j$ for $1\le j\le d$ which are defined by $\boldsymbol{v}_i\cdot\boldsymbol{k}_j=2\pi\delta_{ij}$, where we denote the Kronecker delta by δ_{ij}. Then the first Brillouin zone is given by $B=\left\{\sum_{j=1}^d \xi_j\boldsymbol{k}_j, \xi_j\in[-1/2,1/2]\right\}$.

The asymptotic behavior of the solution ψ^ε 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 $\dot{\boldsymbol{r}}=\partial_{\boldsymbol{k}}E_m(\boldsymbol{k})$, $\dot{\boldsymbol{k}}=-\partial_{\boldsymbol{r}}U$, where E_m is the energy corresponding to the m-th *Bloch band* [9], and U is the external potential. This result has been justified both from a physical point of view in, *e.g.* [4,42], and from a mathematical point of view in, *e.g.* [6,7,18,30]. Higher order corrections relevant to the Berry phase can be included, see *e.g.* [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 ε 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 [39], semiconductors to Bose-Einstein condensation [10]. Mathematical studies on band-crossings can be found in *e.g.* [20,26,29]. One of the most interesting applications of (1.1) is when Γ has