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FAST HUYGENS SWEEPING METHODS FOR SCHRÖDINGER EQUATIONS IN THE SEMI-CLASSICAL REGIME*

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Abstract. We propose fast Huygens sweeping methods for Schrödinger equations in the semi-classical regime by incorporating short-time Wentzel-Kramers-Brillouin-Jeffreys (WKBJ) propagators into Huygens' principle. Even though the WKBJ solution is valid only for a short time period due to the occurrence of caustics, Huygens' principle allows us to construct the global-in-time semi-classical solution. To improve the computational efficiency, we develop analytic approximation formulas for the short-time WKBJ propagator by using the Taylor expansion in time. These analytic formulas allow us to develop two classes of fast Huygens sweeping methods, among which one is posed in the momentum space, and the other is posed in the position space, and both of these methods are of computational complexity $O(N \log N)$ for each time step, where N is the total number of sampling points in the d-dimensional position space. To further speed up these methods, we also incorporate the soft-thresholding sparsification strategy into our new algorithms so that the computational cost can be further reduced. The methodology can also be extended to nonlinear Schrödinger equations. One, two, and three dimensional examples demonstrate the performance of the new algorithms.

Key words. Fast Huygens sweeping method, eikonal equation, WKBJ, convolution, fast Fourier transform, Schrödinger equation.

AMS subject classifications. 65N30, 65M60.

1. Introduction.

Consider the Schrödinger equation for a particle with unity mass

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)U \equiv i\hbar\, U_t - V(x)U + \frac{\hbar^2}{2}\Delta U = 0, \quad x \in \mathcal{R}^d, \quad t > t_0, \tag{1.1}$$

$$U(x,t_0) = U_{t_0}(x) \tag{1.2}$$

where $H = -\frac{\hbar^2}{2}\Delta + V(x)$, the potential V is real and smooth, and $\hbar \equiv h/2\pi$ with h a small (scaled) Planck's constant. When $\hbar$ is small, the wave function $U(x,t)$ for the Schrödinger equation is highly oscillatory, and it is very costly to apply direct methods such as finite-difference methods to compute these wave functions as such methods require very fine meshes to resolve oscillations generated by the equation. Therefore, alternative methods such as asymptotic methods are sought to resolve these highly oscillatory wave functions in the semi-classical regime, where semi-classical refers to an asymptotic theory in which one part of a system is described quantum-mechanically whereas the other, such as a particle trajectory, is treated classically. In this paper, we propose novel methods, called fast Huygens sweeping methods, for solving the Schrödinger equation in the semi-classical regime by incorporating the short-time Wentzel-Kramers-Brillouin-Jeffreys (WKBJ) propagator into Huygens' principle.

To develop these new methods, we utilize the following WKBJ ansatz for the quantum wave function,

$$U(x,t) \approx A(x,t)\exp\left(\frac{i\,\tau(x,t)}{\hbar}\right), \tag{1.3}$$

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