Schrodinger Equation Liouville Equation

### Lab Session

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# Problem I



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#### Consider Schrodinger equation

$$i\epsilon\phi_t = -\frac{\epsilon^2}{2}\Delta\phi + V(x)\phi$$
 (1)

$$\phi(x,0) = \phi_0(x) \tag{2}$$

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and physical observables

$$\rho(x,t) = |\phi(x,t)|^2 \text{ position density}$$
(3)  
$$J(x,t) = \epsilon \operatorname{Im}(\overline{\phi(x,t)}\nabla\phi(x,t)) \text{ current density}$$
(4)

In 1D case,

$$i\epsilon\phi_t = -rac{\epsilon^2}{2}\phi_{xx} + V(x)\phi, \quad a < x < b$$
 (5)

$$\phi(x,0) = \phi_0(x), \quad \phi(a,t) = \phi(b,t), \quad \phi_x(a,t) = \phi_x(b,t)$$
 (6)

Solve this problem with the following schemes:

- Time-Splitting Spectral Method (SP)
- Crank-Nicolson Spectral Method (CNSP)
- Crank-Nicolson Finite Difference Method (CNFD)

If the initial data is given in the WKB form:

$$\phi(x,0) = A_0(x)e^{i\frac{S_0(x)}{\epsilon}}$$
(7)

One can get the semiclassical limit ( $\epsilon \rightarrow 0$ ) by the Wigner transform,

$$W_t + v \cdot \nabla_x W - \nabla_x V \cdot \nabla_v W = 0 \tag{8}$$

$$W(x, v, 0) = \rho_0(x)\delta(v - u_0(x))$$
(9)

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this equation can be solved by the level set method and used as a comparison to the previous methods.

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# Problem II



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Similar as before, by taking the high frequency limit of the wave equation:

$$u_{tt} - c(x)^2 \Delta u = 0 \tag{10}$$

$$u(x,0) = A_0(x)e^{\frac{iS_0(x)}{\epsilon}}$$
(11)

$$u_t(x,0) = B_0(x)e^{\frac{iS_0(x)}{\epsilon}}$$
(12)

one gets the Liouville equation in geometrical optics

$$f_t + H_v \cdot \nabla_x f - H_x \cdot \nabla_v f = 0 \tag{13}$$

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The Hamiltonian *H* is H(x, v) = c(x)|v|, where *v* is the normal slowness vector of the front, c(x) is the local wave speed of the medium.

In 1D case,

$$f_t + c(x) \operatorname{sign}(v) f_x - c_x |v| f_v = 0$$
 (14)

$$f(x, v, 0) = \rho_0(x)\delta(v - u_0(x))$$
(15)

A (1) > A (2) > A

When c(x) has discontinuities due to different media, the waves will undergo partial transmissions and partial reflections.

Use Hamiltonian Preserving scheme to solve this problem. Here level set method doesn't work. Directly evolve the delta function initial data using a upwind scheme.