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PARTICLE METHOD FOR THE WIGNER EQUATION IN HIGH-FREQUENCY PARAXIAL PROPAGATION

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1.INTRODUCTION.

The parabolic wave equation (Schrödinger equation), is an approximation to the Helmholtz equation, which has applications to many different wave propagation problems arising in science and engineering. It seems to appear for first time in the work of Leontovich and Fock [FO] (see also [Fl], [BB], [BK])in the mid-1940's, who they applied the method to describe the propagation of electromagnetic waves along the surface of the earth. Later parabolic approximation method was applied to many other fields, like in plasma physics, for the study of beam propagation [TAP2], in seismology for understanding seismic waves in earth's crust, in laser optics ("quasi-optical" equation method), and in the investigation of random waves [TAT1]. Another important field where parabolic approximation has been established as a fundamental tool is underwater acoustics. At the beginning the method was introduced by Tappert [TAP1] for modeling and computing low-frequency, long-range propagation of sound waves in the ocean, but now the method is used for computations to much higher frequencies.

In this work we address the problem of paraxial propagation in relatively high frequencies (or equivalently, by rescaling, for large Fresnel numbers). Our approach is based on the use of Wigner equation in phase space. A first attempt for the numerical solution of this equation for some simple basic examples is performed by the method of particles. The Wigner transform has been introduced since 1932, as an alternative to non-existing joint probability densities in quantum theory [WIG](see also [TAT2]). It has not received much attention in Applied Mathematics literature, until very recently when Markowich [GM], [GMMP] employed this equation for analyzing semiconductor devices and related wave problems, and Papanicolaou [PR] used the Wigner transform for investigating waves in random media and rigorously constructing radiation transport equations. Even more recently Perthame [BKP], [RP] attempted to apply the Wigner transform for the high frequency Helmholtz equation with source term. However, the Wigner distribution (implicitly or explicitly) has been used in heuristic studies of classical waves since seventies. For example,Tappert [TAP2] has essentially used the Wigner distribution for performing diffractive ray tracing of laser beams and he has proposed a "quasiparticle" representation for possible numerical treatment. An interesting review on the "quasiparticle view" of wave propagation until 1980 has been presented by Marcuvitz [MA]. For later and much more mathematical developments, someone should refer to Lions and Paul [LP] and Papanicolaou and Ryzhik [PR].

The contents of the work are as follows. In Section 2 we present the basics of the parabolic equation. In Section 3 we introduce the Wigner transform and its basic properties, and we derive the Wigner equation for the Schrödinger equation. Finally, in Section 4 we present the particle method for the Wigner equation and we solve numerically two examples (harmonic oscillator and potential barrier). The numerical results of the particle method are well compared with a FEM solution for intermediate frequencies. However, for very high frequencies the FEM solution seems to be inaccurate and it cannot be improved, while the particle solution needs a tremendous big number of particles in order to be in reasonable agreement with the available analytical solution for the harmonic oscillator. A similar situation appears in the case of a potential barrier where non analytical solution is available.

2.PARAXIAL APPROXIMATION.

2.1 Physical conditions.

The parabolic approximation method (more precisely, paraxial approximation), as is applied to the long-range propagation of acoustic signals in the ocean, is based on the special propagation features of sound channel mode of propagation (guided waves), which makes possible this phenomenon. Sound channel propagation takes place in a waveguide that is relatively thin in the vertical direction, and greatly enlogated horizontally, and which confines the acoustic waves within the water column and prevents their interaction with the bottom.

Comparing the approximation under discussion with the other two basic approximating methods in underwater acoustics, that is geometrical acoustics and normal-mode expansions, we can observe its advantages. Geometrical acoustics methods need small wavelengths in order to have negligible diffraction effects, and separation of variables methods are valid only in an exactly horizontally stratified ocean. Though, parabolic approximation methods retain diffraction effects and are valid for more realistic oceans, where horizontal variation of the refraction index is allowed.

The fact that the largest angles of interest in long range propagation are rather small sets the stage of the parabolic approximation. In order to explain why long range propagation corresponds essentially to small angles of propagation, we use the geometrical acoustics for a horizontally stratified ocean, and we assume that all bottom interacting rays are attenuated rapidly enough, so that they don't contribute to long range propagation. Indeed, by Snell's law, the maximum angle of propagation, with respect to the horizontal direction, is given by

$$\theta_l = \cos^{-1}\Big(\frac{c_{min}}{c_{max}}\Big) \ , \tag{2.1.1}$$

where c_{min}, c_{max} are the extreme values of the sound speed in the ocean. For the derivation of (2.1.1) we consider the Hamiltonian

$$H(x,z,k_x,k_z) = \frac{1}{2}(\mathbf{k}^2 - \eta^2(z)) \ , \qquad k^2 = k_x^2 + k_z^2 \ ,$$

corresponding to the Helmholtz equation with refraction index $\eta(z)$. The rays (characteristics) emanating from $x = z = 0$, are found from the corresponding Hamiltonian system

$$\begin{cases} \dfrac{dx}{dt} = k_x, \ \dfrac{dz}{dt} = k_z \\ \dfrac{dk_x}{dt} = 0, \ \dfrac{dk_z}{dt} = (\eta^2(z)/2)' \\ x(0) = 0, \ z(0) = 0 \\ k_x(0) = k_{x_0}, \ k_z(0) = k_{z_0} \ . \end{cases} \tag{2.1.2}$$

Solving this system we obtain

$$k_z^2 = k_{z_0}^2 - \eta^2(0) + \eta^2(z) \ ,$$

and

$$\Big(\frac{dz}{dx}\Big)^2 = \frac{k_z^2}{k_{x_0}^2} \ .$$

At the bottom depth $z = z_b$, we want $k_z \mid_{z=z_b} = 0$, and noting that $\frac{dz}{dx} = sin\theta$, $\theta_b = 0$ we have

$$cos\theta_l = \big(1 - sin^2\theta_l\big)^{1/2} = \Big(1 - \big(\frac{k_{z_0}}{\mathbf{k}^2(0)}\big)^2\Big)^{1/2} = \frac{\eta(z_b)}{\eta(0)} = \frac{\frac{c_0}{c_{max}}}{\frac{c_0}{c_{min}}}$$

which gives us (2.1.1).

Moreover, if we put $\Delta c = c_{max} - c_{min}$, where c_0 is an average sound speed, then

$$\frac{c_{min}}{c_{max}} = 1 - \frac{\Delta c}{c_{max}} \ ,$$

and using

$$cos(\theta_l) \approx 1 - \frac{\theta_l^2}{2}$$

for small θ_l, we find

$$\theta_l \approx \frac{2\Delta c}{c_{max}} \approx \frac{2\Delta c}{c_0}$$

Typically, in the ocean $c_0 \approx 1500m/sec$ and $\Delta c/c_0 \precsim 0.04$, and therefore $\theta_l \precsim 16^o$. This is the reason that sometimes the parabolic equation we will derive in the sequel is called the 16^o-approximation in physics and engineering literature.

2.2 Derivation of the parabolic wave equation.

We proceed now to the derivation of the parabolic wave equation for realistic ocean environments, which even though they may not be analytically solvable, are especially well adapted for numerical computations.

We consider a fixed point source at $x = y = 0$, $z = z_s$ which radiates a spherical wave at fixed frequency ω, and we assume that the refraction index of the ocean depends on all three spatial coordinates, but not on time. We also assume that the density of the fluid is constant, and that the volume attenuation is zero.

Then, the complex acoustic pressure satisfies the Helmholtz equation, which in cylindrical coordinates $(r, \phi, z)$is written in the form

$$\Delta p + k_0^2 \eta^2(z, r, \phi) p = -\delta(\vec{x}) \ , \tag{2.2.1}$$

where

$$\Delta p = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial p}{\partial r}) + \frac{\partial^2 p}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 p}{\partial \phi^2}$$

is the Laplacian, and

$$\delta(\vec{x}) = \frac{1}{2\pi r}\delta(z - z_s)\delta(r) \ ,$$

is the Dirac function in cylindrical coordinates. Here $k_0 = \frac{\omega}{c_0}$, is the wavenumber,ω is the angular acoustic frequency and $\eta(z, r, \phi) = c_0/c(z, r, \phi)$ is the refraction index, both corresponding to a reference sound speed c_0.

For solving equation (2.2.1) we must determine the boundary conditions on the surface $z = 0$ and the bottom of the ocean. As surface boundary condition is traditionally used the pressure release condition $p(z = 0, r, \phi) = 0$. The bottom boundary condition depends on the modeling the bottom. Generally waves that penetrate deep into the subbottom layers do not contribute significantly to long range propagation and should be removed from the calculation. This effect is sometimes modeled by complexifying the refraction index as $\eta^2(z, r, \phi) + iv(z, r, \phi)$, where v increase rapidly for z much greater than the depth of the ocean and then cutting off the calculational domain at a depth where the acoustic field has been reduced to a negligible amplitude. However, such a modeling is not always consistent with the underlying continuum mechanics, and rigorous boundary conditions assuming fluid, elastic or poroelastic bottoms can be devised in the expense of complication of the numerical treatment of the problem.

Moreover, radiation conditions of Sommerfeld type must be prescribed for $r \to \infty$ to guarantee uniqueness of the solution of the Helmholtz equation (cf. [GX], [XU]). and they will be built in the asymptotic decomposition of the pressure field below (cf. eq. (2.2.2)).

For the case that we are assuming that all significant acoustic waves are propagating mostly in the horizontal direction away from the source, the acoustic field may be represented as

$$p(z,r,\phi) = \psi(z,r,\phi) H_0^{(1)}(k_0 r) \tag{2.2.2}$$

where $H_0^{(1)}(k_0 r)$ is the Hankel function of zero order and first kind (outgoing radial solution of the Helmholtz equation in cylindrical coordinates), and ψ is an envelope function that depends on depth, range and azimuth. The above representation is expected to be a good approximation only when $k_0 r >> 1$. For low frequencies this conditions holds in the far field of the point source, but for higher frequencies the range of validity may be reduced. Also, since the representation (2.2.2) is not expected to hold near the source, the source term at equation (2.2.1) will be ommited, and we will consider the homogeneous Helmholtz equation

$$\Delta p + k_0^2 \eta^2(z,r,\phi) p(z,r,\phi) = 0 \ . \tag{2.2.3}$$

In order to derive an equation for the envelope ψ we substitute (2.2.2) into (2.2.3). First we compute

$$\begin{aligned}
&\Delta(\psi H_0^{(1)}(k_0 r)) = \\
&= \frac{\partial^2 \psi}{\partial r^2} H_0^{(1)}(k_0 r) + \left(\frac{2\partial(H_0^{(1)}(k_0 r))}{\partial r} + \frac{1}{r} H_0^{(1)}(k_0 r) \right) \frac{\partial \psi}{\partial r} + \\
&+ \frac{\partial^2 \psi}{\partial z^2} H_0^{(1)}(k_0 r) + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \phi^2} H_0^{(1)}(k_0 r) + \frac{1}{r} \frac{\partial(H_0^{(1)}(k_0 r))}{\partial r} \psi + \frac{\partial^2}{\partial r^2}(H_0^{(1)}(k_0 r)) \psi \ .
\end{aligned}$$

Then, we have

$$\begin{aligned}
&\left(\Delta(\psi H_0^{(1)}(k_0 r)) + k_0^2 \eta^2 (\psi H_0^{(1)}(k_0 r)) \right) \frac{1}{H_0^{(1)}(k_0 r)} = \\
&= \frac{\partial^2 \psi}{\partial r^2} + \left(\frac{2}{H_0^{(1)}(k_0 r)} \frac{\partial H_0^{(1)}(k_0 r)}{\partial r} + \frac{1}{r} \right) \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \phi^2} + \\
&+ \left(\frac{1}{r} \frac{1}{H_0^{(1)}(k_0 r)} \frac{\partial H_0^{(1)}(k_0 r)}{\partial r} + \frac{1}{H_0^{(1)}(k_0 r)} \frac{\partial^2 H_0^{(1)}(k_0 r)}{\partial r^2} \right) \psi + k_0^2 \eta^2 \psi = 0 \ ,
\end{aligned}$$

which gives

$$\frac{\partial^2 \psi}{\partial r^2} + \left(\frac{2}{H_0^{(1)}(k_0 r)} \frac{\partial H_0^{(1)}(k_0 r)}{\partial r} + \frac{1}{r} \right) \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} + + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \phi^2} + k_0^2 \big(\eta^2 - 1\big) \psi = 0 \ . \tag{2.2.4}$$

Now, for $k_0 r >> 1$, by the asymptotics of the Hankel function we have

$$H_0^{(1)}(k_0 r) \sim \big(\frac{2}{i \pi k_0 r}\big)^{1/2} e^{i k_0 r} \ ,$$

and

$$\frac{\partial H_0^{(1)}(k_0 r)}{\partial r} = \left(\frac{2}{i\pi k_0 r}\right)^{1/2} e^{ik_0 r}\left(-\frac{1}{2r} + ik_0\right) ,$$

and thus

$$\frac{2}{H_0^{(1)}(k_0 r)}\frac{\partial H_0^{(1)}(k_0 r)}{\partial r} + \frac{1}{r} = 2ik_0\left(1 + O\big(\frac{1}{k_0^2 r^2}\big)\right) .$$

Consequently neglecting the terms of order $1/k_0^2 r^2$, equation (2.2.4) reduces to

$$\frac{\partial^2\psi}{\partial r^2} + 2ik_0\frac{\partial\psi}{\partial r} + \frac{\partial^2\psi}{\partial z^2} + + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + k_0^2\big(\eta^2 - 1\big)\psi = 0 . \tag{2.2.5}$$

If the main radial dependence of the acoustic field is $e^{ik_0 r}$ for some k_0, then the envelope function ψ will vary slowly as a function of r in the wavelength scale, that is

$$\frac{\partial\psi}{\partial r} << k_0\psi ,$$

and therefore we can neglect the term $\frac{\partial^2\psi}{\partial r^2}$ in (2.2.5) with a small error. This leads to the desired approximation, and the parabolic wave equation reads as follows

$$2ik_0\frac{\partial\psi}{\partial r} + \frac{\partial^2\psi}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + k_0^2\big(\eta^2 - 1\big)\psi = 0 . \tag{2.2.6}$$

In the case that the variation of the ocean in azimuth is very gradual, we may omit the scattering in the horizontal azimuthal direction, that is to neglect the term $\partial^2\psi/\partial\phi^2$ in (2.2.6), which means that we consider $\psi = \psi(r,z)$.

Then the parabolic equation becomes

$$i\frac{\partial\psi(z,r)}{\partial r} + \frac{1}{2k_0}\frac{\partial^2}{\partial z^2}\psi(z,r) + \frac{k_0}{2}\Big(\eta^2(z,r) - 1\Big)\psi(z,r) = 0 . \tag{2.2.7}$$

The last equation has the form of the standard Schrödinger equation

$$i\epsilon\partial_t\psi_\epsilon = -\frac{\epsilon^2}{2}\partial_z^2\psi_\epsilon + V(z,t)\psi_\epsilon(z,t) , \tag{2.2.8}$$

with the correspondence

$$\epsilon = 1/k_0 , \qquad t = r , \qquad V(z,t) = \big(\eta^2 - 1\big)/2 , \tag{2.2.9}$$

that is, the range r plays the role of time, and the potential may depend both on space z and time t, which makes the problem quite different from the corresponding quantum mechanical scattering equation.

Equation (2.2.7) is the most widely used parabolic wave equation in underwater acoustics. Other approximations like wide-angle parabolic equation have been devised, which are capable of greater propagation angles. In general, a whole hierarchy of paraxial equations can be derived by certain asymptotic approximations of the symbol of the pseudodifferential operator arising in one-way factorization of the Helmholtz equation (cf. [TAP1], [LEE]).

The initial data for equation (2.2.7) are modeled on the basis of a near source expansion of the solution of the Helmholtz equation (2.2.1), see, e.g., [COL]. However, a systematic asymptotic derivation of the initial conditions for (2.2.7) is still lacking.

2.3 Geometrical acoustics and parabolic approximation.

Observing that equation (2.2.7) is a wave-type equation , we can perform a geometrical acoustics approximation. Therefore, in order to ensure the validity of the parabolic approximation we shall compare the geometrical acoustics approximation [BLP], [KO1], [KO2] of the parabolic wave equation and that of the Helmholtz equation.

We assume that the ocean is horizontally stratified. Then, the index of refraction depends only on depth. i.e. $\eta = \eta(z)$. We also assume that the acoustic frequency is high enough so that we can perform the geometrical acoustics approximation. The Hamiltonian for the Helmholtz equation is given by

$$H(z, r, k_z, k_r) = \frac{1}{2}(\mathbf{k}^2 - \eta^2(z)) \ , \qquad \mathbf{k} = (k_z, k_r) \ ,$$

and the exact ray equations are given by the corresponding Hamiltonian system

$$\begin{aligned} \frac{dr}{dt} &= k_r, \quad \frac{dk_r}{dt} = 0 \\ \frac{dz}{dt} &= k_z, \quad \frac{dk_z}{dt} = (\eta^2(z)/2)' \ . \end{aligned}$$

From this system it follows $k_r =$ constant, and

$$\frac{d^2 z}{dr^2} = \frac{1}{s^2}\frac{d}{dz}(\frac{1}{2}\eta^2(z)) \ , \tag{2.3.1}$$

where $s := \eta(z)\cos\theta =$ constant is Snell's invariant. The angle θ between the rays and the horizontal direction r is given by $\tan\theta = k_z/k_r$.

In order to derive the corresponding rays for the parabolic wave equation (2.2.7), we ask for solutions $\psi(z,r)$ in the form

$$\psi(z,r) = A(z,r)e^{i\Phi(z,r)} \ .$$

Substituting this ansatz into the parabolic wave equation (2.2.7), we have

$$\begin{aligned} & i\left(\frac{\partial A(z,r)}{\partial r} + iA(z,r)\frac{\partial \Phi(z,r)}{\partial r}\right) + \\ & + \frac{1}{2k_0}\left(\frac{\partial^2 A(z,r)}{\partial z^2} + 2i\frac{\partial A(z,r)}{\partial z}\frac{\partial \Phi(z,r)}{\partial z} + iA(z,r)\frac{\partial^2 \Phi(z,r)}{\partial z^2} - A(z,r)\left(\frac{\partial \Phi(z,r)}{\partial z}\right)^2\right) + \\ & + \frac{k_0}{2}(\eta^2(z) - 1)A(z,r) = 0 \ . \end{aligned}$$

Equating the real and imaginary parts of the last equation to zero, we obtain the system

$$\frac{\partial A(z,r)}{\partial r} + \frac{1}{k_0}\frac{\partial A(z,r)}{\partial z}\frac{\partial \Phi(z,r)}{\partial z} + \frac{1}{2k_0}A(z,r)\frac{\partial^2 \Phi(z,r)}{\partial z^2} = 0 \ , \tag{2.3.2}$$

$$A(z,r)\frac{\partial \Phi(z,r)}{\partial r} + \frac{1}{2k_0}\frac{\partial^2 A(z,r)}{\partial z^2} - \frac{1}{2k_0}\left(\frac{\partial \Phi(z,r)}{\partial z}\right)^2 A(z,r) + \frac{k_0}{2}(\eta^2(z) - 1)A(z,r) = 0 \ . \tag{2.3.3}$$

Setting

$$\theta(z,r) = \frac{1}{k_0}\frac{\partial \Phi(z,r)}{\partial z} \ ,$$

the equations (2.3.2) and (2.3.3) are written in the form

$$\frac{\partial A^2(z,r)}{\partial r} + \frac{\partial}{\partial z}\left(\theta(z,r)A^2(z,r)\right) = 0 \ , \tag{2.3.4}$$

and

$$\frac{\partial \theta(z,r)}{\partial r} + \theta(z,r)\frac{\partial \theta(z,r)}{\partial z} = \frac{1}{2{k_0}^2}\frac{\partial}{\partial z}\left(\frac{1}{A(z,r)}\frac{\partial^2 A(z,r)}{\partial z^2}\right) + \frac{\partial}{\partial z}\left(\frac{1}{2}\eta^2(z)\right) \ , \tag{2.3.5}$$

respectively.

In performing the geometrical acoustics' approximation, we take the formal limit $k_0 \to \infty$ of (2.3.5), which is approximated by

$$\frac{\partial \theta(z,r)}{\partial r} + \theta(z,r)\frac{\partial \theta(z,r)}{\partial z} = \frac{\partial}{\partial z}\left(\frac{1}{2}\eta^2(z)\right) \ . \tag{2.3.6}$$

Moreover, from (2.3.4) we see that the acoustic power $A^2(z,r)$ is invariantly transported along the characteristic curves

$$\frac{dz}{dr} = \theta(z,r) \ . \tag{2.3.7}$$

Combining (2.3.6) and (2.3.7), we find the following equation for the rays of the parabolic wave equation

$$\frac{d\theta(z,r)}{dr} = \frac{d}{dz}\left(\frac{1}{2}\eta^2(z)\right) \ . \tag{2.3.8}$$

Comparing the ray equations (2.3.1) and (2.3.8), we note that ray equations for the parabolic wave equation are the same as those for the Helmholtz equation with $s = 1$. But in order that $s \sim 1$ we need that $\eta(z) \approx 1$ and $\theta << 1$. This conclusion verifies that small angles of propagation is a necessary condition for the parabolic approximation to be valid.

2.4. The high-frequency regime.

The parabolic equation (2.2.7) has been traditionally used for small frequencies on the basis of a physical argument saying that the volume absorption of sound energy increases very fast with frequency. More recently computations based on the parabolic equation have been used for higher frequencies, in a somehow inconsistent way, but the numerical results seem to be reasonable. On the other hand, the Helmholtz equation (2.2.1) and its approximation (2.2.7) are derived from first principles of mechanics with no dissipation in the basic equations. Dissipation is usually introduced a posteriori by complexifying the frequency, and this corresponds to a particular energy dissipation mechanism which may be not compatible with the underlying continuum mechanics.

Assuming here that there is not any dissipation, we investigate the high frequency case (ϵ small), thus attempting to reduce the range of validity of the numerical computation, and to perform as much as possible "near field" calculations, as the actual parameter entring the derivation of (2.2.7) is $k_0 r$. Moreover, by rescaling the equation (2.2.7) it is always possible to introduce in place of $\epsilon = 1/k_0$, the parameter $\epsilon = 1/F$, $F = k_0 Z^2/R$ being the Fresnel number, with R, Z the characteristic horizontal and vertical distances of the wave field.

3.The Wigner equation.

3.1 The Wigner transform. [PR],[LP]

For any smooth function $\psi(\mathbf{x})$ rapidly decaying at infinity, that is $\psi \in \mathcal{S}(\mathbb{R})$, the Wigner transform of ψ is a quadratic transform defined by

$$W[\psi](x,k) = W(x,k) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy \tag{3.1.1}$$

where $\overline{\psi}$ is the complex conjugate of ψ. The Wigner transform is a defined in phase space $\mathbb{R}_{xk}$, it is real, and it has many important properties, the most remarkable of them being the following.

First, the k-integral of $W(x,k)$ is the energy density of ψ

$$\int_{\mathbb{R}} W(x,k)dk = |\psi(x)|^2 \ . \tag{3.1.2}$$

In fact, we have

$$\begin{aligned}\int_{\mathbb{R}} W(x,k)dk &= \frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} e^{-iky}\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dydk = \\ &= \int_{\mathbb{R}}\left(\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}dk\right)\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy = \\ &= \int_{\mathbb{R}}\delta(y)\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy = \psi(x)\overline{\psi}(x) = |\psi(x)|^2 \ .\end{aligned}$$

Here δ is the δ-function, and we used the Fourier transform $\delta(y) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}dk$.

Second, the first moment in k of $W(x,k)$ is the energy flux

$$\int_{\mathbb{R}} kW(x,k)dk = \frac{1}{2i}(\psi(x)\overline{\psi^{'}}(x) - \overline{\psi}(x)\psi^{'}(x)) = \mathcal{F}(x) \ . \tag{3.1.3}$$

In fact, we have

$$\begin{aligned}\int_{\mathbb{R}} kW(x,k)dk = \int_{\mathbb{R}}\left(\frac{1}{2\pi}\int_{\mathbb{R}} ke^{-iky}dk\right)\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy = -\frac{1}{i}\int_{\mathbb{R}}\delta^{'}(y)\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy = \\ =\frac{1}{i}\int_{\mathbb{R}}\delta(y)\left(\frac{1}{2}\psi^{'}(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2}) - \frac{1}{2}\overline{\psi^{'}}(x-\frac{y}{2})\psi(x+\frac{y}{2})\right)dy = \\ =\frac{1}{2i}\left(\overline{\psi}(x)\psi^{'}(x) - \psi(x)\overline{\psi^{'}}(x)\right).\end{aligned}$$

The x to k duality in phase space can be recognized using the alternative definition

$$W(x,k) = \int_{\mathbb{R}} e^{ipx}\widehat{\psi}(-k-\frac{p}{2})\overline{\widehat{\psi}(-k+\frac{p}{2})}dp \ , \tag{3.1.4}$$

where $\widehat{\psi}(k) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{ikz}\psi(z)dz$ denotes the Fourier transform of ψ.

In fact, the definitions (3.1) and (3.2) are equivalent, since we have

$$\begin{aligned}
W(x,k) =&\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\psi(x+\frac{y}{2})\overline{\psi}(x-\frac{y}{2})dy = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\int_{\mathbb{R}} e^{-iz(x+\frac{y}{2})}\widehat{\psi}(z)dz\overline{\int_{\mathbb{R}} e^{-iw(x-\frac{y}{2})}\widehat{\psi}(w)dw}dy = \\
=&\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\int_{\mathbb{R}} e^{-iz(x+\frac{y}{2})}\widehat{\psi}(z)dz\int_{\mathbb{R}} e^{iw(x-\frac{y}{2})}\overline{\widehat{\psi}}(w)dwdy = \\
=&\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iy(k+\frac{z}{2}+\frac{w}{2})}dy\right)e^{-i(z-w)x}\widehat{\psi}(z)\overline{\widehat{\psi}}(w)dzdw = \\
=&\int_{\mathbb{R}}\int_{\mathbb{R}}\delta(k+\frac{z}{2}+\frac{w}{2})e^{-i(z-w)x}\widehat{\psi}(z)\overline{\widehat{\psi}}(w)dzdw = \\
=&2\int_{\mathbb{R}} e^{-i2(k+z)x}\widehat{\psi}(z)\overline{\widehat{\psi}}(-2k-z)dz = \int_{\mathbb{R}} e^{ipx}\widehat{\psi}(-k-\frac{p}{2})\overline{\widehat{\psi}}(-k+\frac{p}{2})dp = \\
=&\int_{\mathbb{R}} e^{ipx}\widehat{\psi}(-k-\frac{p}{2})\overline{\widehat{\psi}}(-k+\frac{p}{2})dp \ .
\end{aligned}$$

In the case of high frequency wave propagation, the WKB method suggests solutions of the form

$$\psi^\epsilon(x,t) = e^{iS(x,t)/\epsilon}A(x,t) \ , \qquad \epsilon\to 0 \ ,$$

where S is a real-valued and smooth phase, and A is a real-valued smooth amplitude of compact support. The Wigner distribution of $\psi^\epsilon(x)$ is

$$W(x,k) = \frac{1}{2\pi}\int_R e^{-iky}e^{iS(x+\frac{y}{2})/\epsilon}A(x+\frac{y}{2})e^{-iS(x-\frac{y}{2})/\epsilon}\overline{A}(x-\frac{y}{2})dy \ ,$$

but $W(x,k)$ does not converge as $\epsilon\to 0$. However, it can be shown that the rescaled version of $W(x,k)$,

$$W^\epsilon(x,k) = \frac{1}{\epsilon}W(x,\frac{k}{\epsilon})$$

converges weakly as $\epsilon\to 0$ [PR], [LP].

Indeed, proceeding formally, we rewrite W^ϵ in the form

$$W^\epsilon(x,k) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}A(x+\frac{\epsilon y}{2})\overline{A}(x-\frac{\epsilon y}{2})e^{\frac{i}{\epsilon}\left[S(x+\frac{\epsilon y}{2})-S(x-\frac{\epsilon y}{2})\right]}dy \ ,$$

and we expand in Taylor series about $y=0$ both A and S. Then, we have

$$\begin{aligned}
A(x+\frac{\epsilon y}{2})\overline{A}(x-\frac{\epsilon y}{2}) &= \left(A(x)+\frac{\epsilon}{2}yA^{'}(x)+\dots\right)\left(\overline{A}(x)-\frac{\epsilon}{2}y\overline{A}^{'}(x)+\dots\right) \\
&= A(x)\overline{A}(x)+O(\epsilon) = |A(x)|^2+O(\epsilon) \ ,
\end{aligned}$$

and

$$\begin{aligned}
S(x+\frac{\epsilon y}{2})-S(x-\frac{\epsilon y}{2}) = &\left(S(x)+\frac{\epsilon}{2}yS^{'}(x)+\frac{\epsilon^2}{4}S^{''}(x)+\dots\right)-\left(S(x)-\frac{\epsilon}{2}yS^{'}(x)+\frac{\epsilon^2}{4}S^{''}(x)-\dots\right) = \\
= &\epsilon yS^{'}(x)+O(\epsilon^3) \ .
\end{aligned}$$

Retaining only terms of order $O(1)$ in A and $O(y)$ in S, and integrating the expansion termwise we obtain that $W^\epsilon(x,k)$ "converges" to

$$W(x,k) = |A(x)|^2 \frac{1}{2\pi}\int_{\mathbb{R}} e^{-i(k-S'(x))y}dy = |A(x)|^2\delta(k-S'(x)) \ , \tag{3.1.5}$$

which is a Dirac measure, concentrated on the Lagrangian manifold $k = S'(x)$, associated with the phase of the WKB solution ψ^ϵ [ARN1],[ARN2], and it is the correct weak limit [LP]. More precisely, if Q is any test function in $\mathcal{S}(\mathbb{R}^2)$, then

$$\int_{\mathbb{R}}\int_{\mathbb{R}} Q(x,k)W^\epsilon(x,k)dxdk \to \int_{\mathbb{R}} Q(x,S'(x))|A(x)|^2 dx \ .$$

The above observations suggest that the scaled Wigner transform

$$\begin{aligned} W^\epsilon(x,k) &= \frac{1}{\epsilon}W(x,\frac{k}{\epsilon}) = \\ &= \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\psi^\epsilon(x+\frac{\epsilon y}{2})\overline{\psi}^\epsilon(x-\frac{\epsilon y}{2})dy \ , \end{aligned} \tag{3.1.6}$$

is the correct phase-space object for analyzing high frequency waves.

3.2 The Wigner equation for the Schrödinger equation.

We consider the following initial-value problem for the Schrödinger equation (cf. eq. (2.2.8)), with time-independent potential (this corresponds to range-independent ocean sound speed)

$$\begin{cases} i\epsilon\partial_t\psi^\epsilon(x,t) = -\dfrac{\epsilon^2}{2}\partial_x^2\psi^\epsilon(x,t) + V(x)\psi^\epsilon(x,t) \\ \psi^\epsilon(x,0) = \psi_0^\epsilon(x,t) \ . \end{cases} \tag{3.2.1}$$

Let $W^\epsilon(x,k,t)$ be the scaled Wigner distribution of $\psi^\epsilon(x,t)$. In order to find the equation that $W^\epsilon(x,k,t)$ satisfies, we start with the identity

$$\begin{aligned} & i\epsilon\left(\partial_t\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) + \partial_t\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t)\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\right) = \\ & = -\frac{\epsilon^2}{2}\left(\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t)\partial_x^2\psi^\epsilon(x+\frac{\epsilon}{2}y,t) - \psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x^2\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t)\right) + \\ & + \left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right)\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) \ . \end{aligned} \tag{3.2.2}$$

If we put

$$v^\epsilon(x,y,t) = \psi^\epsilon\big(x+\frac{\epsilon}{2}y,t\big)\overline{\psi_\epsilon}\big(x-\frac{\epsilon}{2}y,t\big)$$

then, we have

$$\partial_x v^\epsilon = \partial_x\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) + \psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) \ ,$$

and

$$\begin{aligned} \partial_y\partial_x v^\epsilon &= \frac{\epsilon}{2}\partial_x^2\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) - \frac{\epsilon}{2}\partial_x\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) \\ &+ \frac{\epsilon}{2}\partial_x\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x\overline{\psi}^\epsilon(x-\frac{\epsilon}{2}y,t) - \frac{\epsilon}{2}\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x^2\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) \\ &= \frac{\epsilon}{2}\left(\partial_x^2\psi^\epsilon(x+\frac{\epsilon}{2}y,t)\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t) - \psi^\epsilon(x+\frac{\epsilon}{2}y,t)\partial_x^2\overline{\psi_\epsilon}(x-\frac{\epsilon}{2}y,t)\right) \ . \end{aligned}$$

Using the above two relations we rewrite (3.2.2) in terms of v^ϵ as follows

$$\begin{aligned} i\epsilon\partial_t v^\epsilon &= -\frac{\epsilon^2}{2}\frac{2}{\epsilon}\partial_y\partial_x v^\epsilon + \left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) v^\epsilon \\ &= -\epsilon\partial_y\partial_x v^\epsilon + \left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) v^\epsilon \ . \end{aligned}$$

Multiplying the last equation by $e^{-iky}/2\pi$, and integrating with respect to y we get

$$\begin{aligned} i\epsilon\partial_t \left\{\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky} v^\epsilon(x,y,t)dy\right\} &= -\epsilon\partial_x\left\{\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\partial_y v^\epsilon(x,y,t)dy\right\} \\ &+ \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) v^\epsilon(x,y,t)dy \ . \end{aligned}$$

By noting that

$$W^\epsilon(x,k,t) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky} v^\epsilon(x,y,t)dy \ ,$$

the above equation is written in the form

$$\begin{aligned} i\epsilon\partial_t W^\epsilon(x,k,t) = &-\epsilon\frac{\partial}{\partial_x}\left\{\frac{1}{2\pi}\left[e^{-iky}v^\epsilon\right]_{-\infty}^{+\infty} + (ik)\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky} v^\epsilon(x,y,t)dy\right\} + \\ &\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) v^\epsilon(x,y,t)dy \ . \end{aligned}$$

Assuming now that $\psi^\epsilon(x,t)$ decays fast enough as $\mid x \mid\to\infty$, we have

$$\lim_{|y|\to+\infty}(e^{-iky}v^\epsilon) = 0 \ ,$$

and therefore W^ϵ satisfies the equation

$$\partial_t W^\epsilon(x,k,t) = -k\partial_x W^\epsilon(x,k,t) + I \ , \tag{3.2.3}$$

where

$$I(x,k,t) = \frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) v^\epsilon(x,y,t)dy \ .$$

Since $W^\epsilon(x,k,t)$ is the Fourier transform of $v^\epsilon(x,y,t)$, we have

$$v^\epsilon(x,y,t) = \int_{\mathbb{R}} e^{i\xi y} W^\epsilon(x,\xi,t)d\xi \ ,$$

and we write I as follows

$$\begin{aligned} I =&\frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} e^{-iky}e^{i\xi y} W^\epsilon(x,\xi,t)\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) d\xi dy = \\ =&\frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}} W^\epsilon(x,\xi,t)\left(\int_{\mathbb{R}} e^{-i(k-\xi)y}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) dy\right) d\xi \ . \end{aligned}$$

Now we define $Z^\epsilon(x,k)$ by

$$Z^\epsilon(x,k) = \frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) dy \ , \tag{3.2.4}$$

and we rewrite I as the convolution

$$I = Z^{\epsilon}(x,k) *_k W^{\epsilon}(x,k,t) \ .$$

Therefore, equation (3.2.3) takes the form of the integrodifferential equation

$$\partial_t W^{\epsilon}(x,k,t) + k\partial_x W^{\epsilon}(x,k,t) - Z^{\epsilon}(x,k) *_k W^{\epsilon}(x,k,t) = 0 \tag{3.2.5}$$

which is known as the Wigner equation.

The Wigner equation (3.2.5) can be written in an alternative form revealing the underlying competition between the hyperbolic and dispersive character in this equation, depending on the value of the frequency ϵ. Expanding in Taylor series the potential V we observe that for small ϵ and fixed x, y we have

$$\frac{1}{\epsilon}\left(V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)\right) = yV^{'}(x) + O(\epsilon) \ .$$

Then, we write $Z^{\epsilon}(x,k)$ in the form

$$Z^{\epsilon}(x,k) = -\frac{i}{2\pi}\int_{\mathbb{R}} e^{-iky}\left[\frac{V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)}{\epsilon} + yV^{'}(x) - yV^{'}(x)\right] dy \ ,$$

that is

$$Z^{\epsilon}(x,k) = J(x,k) + \mathcal{Q}^{\epsilon}(x,k) \ , \tag{3.2.6a}$$

where

$$J(x,k) := \left(-\frac{i}{2\pi}\int_{\mathbb{R}} e^{-iky} y dy\right) V^{'}(x) = \partial_k\left(\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky} dy\right) V^{'}(x) = \delta^{'}(k)V^{'}(x) \ , \tag{3.2.6b}$$

and

$$\mathcal{Q}^{\epsilon}(x,k) := -\frac{i}{2\pi}\int_{\mathbb{R}} e^{-iky}\left[\frac{V(x+\frac{\epsilon}{2}y) - V(x-\frac{\epsilon}{2}y)}{\epsilon} - yV^{'}(x)\right] dy \ . \tag{3.2.6c}$$

Thus, using the formula

$$\delta^{'}(k) *_k W^{\epsilon}(x,k,t) = \partial_k W^{\epsilon}(x,k,t) \ ,$$

the Wigner equation is written in the form

$$\partial_t W^{\epsilon}(x,k,t) + k\partial_x W^{\epsilon}(x,k,t) - V^{'}(x)\partial_k W^{\epsilon}(x,k,t) = \mathcal{Q}^{\epsilon}(x,k) *_k W^{\epsilon}(x,k,t) \ . \tag{3.2.7}$$

We observe that the differential operator in left hand side of (3.2.7) is independent of the small parameter ϵ, while the convolution kernel $\mathcal{Q}^{\epsilon}$ in the right hand side is of order $O(\epsilon^2)$ for fixed x, k. Therefore, the formal limit of the Wigner equation as $\epsilon \to 0$ is the equation

$$\partial_t W(x,k,t) + k\partial_x W(x,k,t) - V^{'}(x)\partial_k W(x,k,t) = 0 \ . \tag{3.2.8}$$

This equation is the standard Liouville equation of classical mechanics in phase space, and it is called the limit Wigner equation.

The initial data for the Wigner equation is the Wigner transform

$$W^\epsilon(x,k,0)=W_0^\epsilon(x,k)=W^\epsilon[\psi_0^\epsilon](x,k)\ , \tag{3.2.9}$$

of the initial data $\psi_0^\epsilon(x)=\psi^\epsilon(x,t=0)$. On the other hand, the initial data for the limit Wigner equation are found by taking the limit of $W^\epsilon(x,k,0)$ as $\epsilon\to 0$, and they have the form (cf. Section 3.1)

$$W_0(x,k)=|A_0(x)|^2\delta(k-S_0^{'}(x))\ . \tag{3.2.10}$$

The solution of (3.2.8) is given by

$$W(x,k,t)=|A(x,t)|^2\delta(k-S^{'}(x,t)) \tag{3.2.11}$$

with $S(x,t),\ A(x,t)$ solutions of the eikonal and transport equations, respectively,

$$S_t(x,t)+\frac{1}{2}|S_x(x,t)|^2+V(x)=0\ ,\qquad S(x,t=0)=S_0(x)\ , \tag{3.2.12a}$$

and

$$(|A(x,t)|^2)_t+(|A(x,t)|S_x(x,t))_x=0\ ,\qquad |A(x,t=0)|^2=|A_0(x)|^2\ , \tag{3.2.12b}$$

In fact, differentiating (3.2.11), and using the formula

$$f(k)\delta^{'}(k-k_0)=-f^{'}(k_0)\delta(k-k_0)+f(k_0)\delta^{'}(k-k_0)\ ,$$

we have

$$\begin{aligned}
\partial_t W(x,k,t)&=\partial_t(|A(x,t)|^2)\delta(k-\partial_x S(x,t))-|A(x,t)|^2\partial_x\partial_t S(x,t)\delta^{'}(k-\partial_x S(x,t))\ ,\\
\partial_x W(x,k,t)&=\partial_x(|A(x,t)|^2)\delta(k-\partial_x S(x,t))-\partial_x^2 S(x,t)|A(x,t)|^2\delta^{'}(k-\partial_x S(x,t))\ ,\\
\partial_k W(x,k,t)&=|A(x,t)|^2\delta^{'}(k-\partial_x S(x,t))\ .
\end{aligned}$$

Then,

$$\begin{aligned}
k\partial_x W(x,k,t)&=k\partial_x(|A(x,t)|^2)\delta(k-\partial_x S(x,t))-k\partial_x^2 S(x,t)|A(x,t)|^2\delta^{'}(k-\partial_x S(x,t))=\\
&=\partial_x S(x,t))\partial_x(|A(x,t)|^2)\delta(k-\partial_x S(x,t))+\partial_x^2 S(x,t)|A(x,t)|^2\delta(k-\partial_x S(x,t))\\
&-\partial_x^2 S(x,t)\partial_x S(x,t)\delta^{'}(k-\partial_x S(x,t))\ ,
\end{aligned}$$

and therefore using (3.2.12a) and (3.2.12b) we have

$$\begin{aligned}
&\partial_t W(x,k,t)+k\partial_x W(x,k,t)-V^{'}(x)\partial_k W(x,k,t)=\\
&=\Big(\partial_t(|A(x,t)|^2)+\partial_x S(x,t))\partial_x(|A(x,t)|^2)+\partial_x^2 S(x,t)|A(x,t)|^2\Big)\delta(k-\partial_x S(x,t))-\\
&-|A(x,t)|^2\Big(\partial_x\partial_t S(x,t)+\partial_x^2 S(x,t)\partial_x S(x,t)+V^{'}(x)\Big)\delta^{'}(k-\partial_x S(x,t))\\
&=\Big(\partial_t(|A(x,t)|^2)+\partial_x(|A(x,t)|^2\partial_x S(x,t))\Big)\delta(k-\partial_x S(x,t))-\\
&-|A(x,t)|^2\Big(\partial_x\big(\partial_t S(x,t)+\frac{1}{2}|\partial_x S(x,t)|^2+V(x)\big)\Big)\delta^{'}(k-\partial_x S(x,t))=0\ .
\end{aligned}$$

It must be emphasized that for potentials of the form $V(x) = ax^2 + bx + c$, a, b, c constants, it easily follows that $\mathcal{Q}^\epsilon \equiv 0$, and therefore the Wigner equation coincides with the limit Wigner equation. These potentials are usually referred as non-essential (or non-diffractive) potentials, since the corresponding bicharacteristics are linear. In this case, only the hyperbolic character of the Wigner equation is present, and no dispersion is coming into play.

The usual mathematical analysis of the Wigner equation (3.2.5) relies on semigroup theory in Hilbert spaces, especially in L^2, which is the natural framework of semiclassical mechanics [M]. But this context cannot used in the numerical analysis of the particle method, which needs L^p or $W^{m,p}$ estimates, and therefore the order of convergence is related to the regularity of the potential V [AN].

4.THE PARTICLE METHOD.

4.1. The particle method for the transport equation. (Raviart [RAV])

A well-known method for solving initial value problems for transport equations of the form

$$\begin{cases} \dfrac{\partial u}{\partial t} + \displaystyle\sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i u) + a_0 u = f \ , \qquad x \in \mathbb{R}^n \ , t > 0 \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) \ , \end{cases} \tag{4.1.1}$$

is the method of characteristics. Here $u = u(\mathbf{x}, t), \ a_i = a_i(\mathbf{x}, t), \ f = f(\mathbf{x}, t)$.

The characteristic curves associated with the first order differential operator $\frac{\partial}{\partial t} + \sum_{i=1}^{n} a_i \frac{\partial}{\partial x_i}$ are given as the solutions of the following differential system

$$\begin{cases} \dfrac{d\mathbf{X}}{dt} = a(\mathbf{X}, t), \qquad \mathbf{X} = (X_1, \ldots, X_n) \ , \\ \mathbf{X}(s) = \mathbf{x}, \qquad a = (a_1, \ldots, a_n) \ . \end{cases} \tag{4.1.2}$$

If the coefficients $a_i, \ 0 \le i \le n$ and the data $u_o, \ f$ are sufficiently smooth, the problem (4.1.1) has a unique classical solution, given by

$$\begin{aligned} u(\mathbf{x}, t) =& u_0(\mathbf{X}(0; \mathbf{x}, t)) J(0; , \mathbf{x}, t) exp\left(-\int_0^t a_0(\mathbf{X}(s; \mathbf{x}, t), s) ds \right) + \\ & \int_0^t f(\mathbf{X}(s; \mathbf{x}, t), s) J(s; \mathbf{x}, t) exp\left(-\int_s^t a_0(\mathbf{X}(\sigma; \mathbf{x}, t) d\sigma \right) ds \ , \end{aligned} \tag{4.1.3}$$

where $J(t; \mathbf{x}, s) = det\left(\frac{\partial X_i}{\partial x_j}(t; \mathbf{x}, s) \right)$ is the Jacobian determinant of the transformation

$$\Phi_s^t(\mathbf{x}) = \mathbf{X}(t; \mathbf{x}, s), \quad \text{for all} \ \ s, t \in [0, T] \ .$$

Under weaker regularity assumptions, the solution (4.1.3) can be considered as a weak solution of problem (4.1.1).

In order to construct a particle method for approximating the solution of the problem (4.1.1), it is enough to consider measure solutions (or even distributional solutions) which are defined as follows.

<u>Definition 4.1.1</u> A measure $u \in \mathcal{M}(\mathbb{R}^n \times [0, T[)$ is called a measure solution of (4.1.1) if

$$\begin{aligned} &\langle u, L^* \phi \rangle = \langle f, \phi \rangle + \langle u_0, \phi(\cdot, 0) \rangle \ , \quad \forall \ \phi \in C_0^1(\mathbb{R}^n \times [0, T[) \\ &\text{for } u_0 \in \mathcal{M}(\mathbb{R}^n), \ f \in \mathcal{M}(\mathbb{R}^n \times [0, T]) \ , \end{aligned}$$

where L^* is the formal adjoint of the linear differential operator

$$Lv = \frac{\partial v}{\partial t} + \sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i v) + a_0 v \ .$$

The first step of a particle method for approximating weak solutions of the problem (4.1.1) is to approximate the initial condition u_0 by a linear combination of Dirac measures,

$$u_h^0 = \sum_{j \in J} \alpha_j \delta(\mathbf{x} - \mathbf{x}_j) \ , \tag{4.1.4}$$

for some set $(\mathbf{x}_j, \alpha_j)_{j\in J}$ of points $\mathbf{x}_j \in \mathbb{R}^n$ and weights $\alpha_j \in \mathbb{R}$.

Consequently, the problem we have to solve (consider the case of $f = 0$ for simplicity), is the following

$$\begin{cases} \dfrac{\partial u_h}{\partial t} + \displaystyle\sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i u_h) + a_0 u_h = 0, & x \in \mathbb{R}^n, t > 0 \\ u_h(\cdot, 0) = u_h^0 \ . \end{cases} \tag{4.1.5}$$

Let u_h be a measure solution of the problem (4.1.5), given by

$$u_h = \sum_{j\in J} \alpha_j(t)\delta(\mathbf{x} - \mathbf{X}_j(t)) \ , \tag{4.1.6}$$

where $\mathbf{X}_j(t)$ and $\alpha_j(t)$ are solutions of the differential systems $(j \in J)$

$$\begin{cases} \dfrac{d}{dt}\mathbf{X}_j(t) = a(\mathbf{X}_j(t), t) \\ \mathbf{X}_j(0) = \mathbf{x}_j \ , \end{cases} \tag{4.1.7}$$

and

$$\begin{cases} \dfrac{d}{dt}\alpha_j(t) + a_0(\mathbf{X}_j(t), t)\alpha_j(t) = 0 \\ \alpha_j(0) = \alpha_j \ , \end{cases} \tag{4.1.8}$$

respectively. Hence for all $t \in [0, T]$, $u(\cdot, t)$ is a sum of Dirac masses whose trajectories in the $(\mathbf{x}, t)$ space coincide with the characteristic curves passing through the points $(\mathbf{x}_j, 0)$. Such a measure solution u_h is called a *particle solution* of (4.1.1).

The problem that comes up first, is how to choose u_h^0 that approximates u_0. The simplest procedure for this is the following. We cover $\mathbb{R}^n$ with a uniform mesh of meshsize h, for some small $h > 0$. For all $j = (j_1, \ldots, j_n) \in \mathbb{Z}^n$, let B_j be the cell

$$B_j = \left\{ \mathbf{x} \in \mathbb{R}^n ; \ (j_i - \frac{1}{2})h \le x_i \le (j_i + \frac{1}{2})h, \quad 1 \le i \le n \right\}$$

where $\mathbf{x}_j = (j_i h)_{1\le i\le n}$ is the center of B_j. Then,we set $u_h^0 = \sum_{j\in\mathbb{Z}^n} \alpha_j \delta(\mathbf{x} - \mathbf{x}_j)$ where α_j is an approximation of $\int_{B_j} u_0 dx$, or equivalently $\alpha_j = h^n u_0(\mathbf{x}_j)$.

In order to compute a numerical approximation of $u(\mathbf{x}, t)$ at a point $(\mathbf{x}, t)$, it is more useful to associate with the measure $u_h(\cdot, t)$ a continuous function $u_h^\eta(\cdot, t)$, which will approximate the function $u(\cdot, t)$ for all $t \in [0, T]$. For this we define

$$u_h^\eta(\mathbf{x}, t) = \sum_{j\in\mathbb{Z}} \alpha_j(t)\zeta_\eta(\mathbf{x} - \mathbf{X}_j(t)) \ , \tag{4.1.9}$$

where $\zeta_\eta(\mathbf{x}) = \frac{1}{\eta^n}\zeta\left(\frac{\mathbf{x}}{\eta}\right)$, and $\zeta \in C^0(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$ is a "cut-off" function such that

$$\int_{\mathbb{R}^n} \zeta(\mathbf{x}) d\mathbf{x} = 1.$$

The convergence of the above descripted procedure for small η is asserted by the following theorem.

Theorem 4.1.1

Assume that

i) there exists an integer $k \geq 1$ such that

$$1) \int_{\mathbb{R}^n} \zeta(\mathbf{x}) d\mathbf{x} = 1$$

$$2) \int_{\mathbb{R}^n} \mathbf{x}^\alpha \zeta(\mathbf{x}) d\mathbf{x} = 0, \ \forall \alpha \in \mathbb{N}^n \text{ with } 1 \leq |\alpha| \leq k-1$$

$$3) \int_{\mathbb{R}^n} |\mathbf{x}|^k |\zeta(\mathbf{x})| d\mathbf{x} < +\infty$$

ii) $\zeta \in W^{m,\infty}(\mathbb{R}^n) \cap W^{m,1}(\mathbb{R}^n)$ for some integer $m > n$

iii) For the coefficients $a_i \in C^0(\mathbb{R}^n \times [0,T])$, $0 \leq i \leq n$, $a_1, \ldots, a_n, a_0 + diva \in L^\infty(0,T; W^{l,\infty}(\mathbb{R}^n))$, $l = max(k,m)$. Then, if $u_0 \in W^{l,p}(\mathbb{R}^n))$, there exists a constant $C = C(T) > 0$, such that for all $t \in [0,T]$

$$\|u(\cdot,t) - u_h^\eta(\cdot,t)\|_{L^p(\mathbb{R}^n)} \leq C \left\{ \eta^k \|u_0\|_{k,p,\mathbb{R}^n} + \left(\frac{h}{\eta}\right)^m \|u_0\|_{m,p,\mathbb{R}^n} \right\} . \blacksquare$$

If we replace the assumption (ii) by the the assumption

iv) ζ has compact support and $\zeta \in W^{m,\infty}(\mathbb{R}^n)$ for some integer $m \geq 1$,

then, we have the following convergence theorem

Theorem 4.1.2

Under the assumptions (i),(iii),(iv), if $u_0 \in W^{l,p}(\mathbb{R}^n)$, there exists a constant $C = C(T) > 0$, such that

$$\|u(\cdot,t) - u_h^\eta(\cdot,t)\|_{L^p(\mathbb{R}^n)} \leq C \left\{ \eta^k \|u_0\|_{k,p,\mathbb{R}^n} + (1 + \frac{h}{\eta})^{\frac{n}{q}} \left(\frac{h}{\eta}\right)^m \|u_0\|_{m,p,\mathbb{R}^n} \right\} , \qquad \frac{1}{p} + \frac{1}{q} = 1 . \blacksquare$$

The last theorem does not hold if ζ belongs only to $L^\infty(\mathbb{R}^n)$. But it can be slightly improved for $m = 0, 1$, when ζ has compact support, it is piecewise smooth and it belongs to $W^{m,\infty}(\mathbb{R}^n)$. In this case, we have the following estimate

$$\|u(\cdot,t) - u_h^\eta(\cdot,t)\|_{L^\infty(\mathbb{R}^n)} \leq C \left\{ \eta^k \|u_0\|_{k,\infty,\mathbb{R}^n} + (1 + \frac{\eta}{h})^{n-1} \left(\frac{h}{\eta}\right)^{m+1} \|u_0\|_{m+1,\infty,\mathbb{R}^n} \right\} .$$

From the above theorems it follows that $\frac{h}{\eta}$ must go to zero, as the parameters h and η go also to zero, for the particle approximation to converge. Numerical computations with the particle method for the transport equation and for a symmetric hyperbolic system have been performed by MasGallic et.al. [MG],[MR],[MP].

4.2 The particle method for the Wigner equation.

In this section, we apply the particle method presented in Section 4.1 for solving the Wigner equation (cf. Section 3.2)

$$\begin{aligned}&\partial_t W^\epsilon + \mathbf{k}\partial_{\mathbf{x}} W^\epsilon - V'(\mathbf{x})\partial_{\mathbf{k}} W^\epsilon(\mathbf{x},\mathbf{k},t) = \mathcal{Q}^\epsilon(\mathbf{x},\mathbf{k}) *_{\mathbf{k}} W^\epsilon(\mathbf{x},\mathbf{k},t) \ ,\\ &W^\epsilon(\mathbf{x},\mathbf{k},0) = W_0^\epsilon(\mathbf{x},\mathbf{k}) \ .\end{aligned} \tag{4.2.1}$$

There are two alternative formulations. The first was proposed by Perthame & Katsaounis(personal communication), and the second was introduced by Arnold and Nier [AN](see also [N] for semiconductor device computations). In the first formulation we consider the particles to move along the bicharacteristics of the Liouville operator $\partial_t + \mathbf{k}\partial_{\mathbf{x}} - V'(\mathbf{x})\partial_{\mathbf{k}}$, while in the second along the characteristics of $\partial_t + \mathbf{k}\partial_{\mathbf{x}}$, having $\mathcal{Z}^\epsilon$ in the right hand side of (4.2.1), instead of $\mathcal{Q}^\epsilon$. In the later case the particles move with k =const.

First formulation

We approximate W_0^ϵ by

$$\begin{aligned}&\widetilde{W_0^\epsilon}(q,p) = \sum_{l=1}^{N} \alpha_l^0 \delta(q-q_l)\delta(p-p_l)\\ &\{(q_l,p_l), \quad l=1,\dots,N\} \text{ are arbitrarily chosen initial particles}\end{aligned} \tag{4.2.2}$$

and we substitute the approximation

$$\widetilde{W^\epsilon}(\mathbf{x},\mathbf{k},t) = \sum_{l=1}^{N} \alpha_l(t)\delta(\mathbf{x}-\mathbf{x}_l(q_l,p_l,t))\delta(\mathbf{k}-\mathbf{k}_l(q_l,p_l,t)) \tag{4.2.3.}$$

for W^ϵ into (4.2.1)

In the sequel we will denote $\mathbf{x}_l(t) = \mathbf{x}_l(q_l,p_l,t)$, $\mathbf{k}_l(t) = \mathbf{k}_l(q_l,p_l,t)$. Differentiating (4.2.3) we have

$$\begin{aligned}\partial_t \widetilde{W^\epsilon}(\mathbf{x},\mathbf{k},t) = &\sum_{l=1}^{N} \dot{\alpha}_l(t)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t)) -\\ &-\sum_{l=1}^{N} \alpha_l(t)\dot{\mathbf{x}}_l\delta'(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t)) -\\ &-\sum_{l=1}^{N} \alpha_l(t)\dot{\mathbf{k}}_l\delta(\mathbf{x}-\mathbf{x}_l(t))\delta'(\mathbf{k}-\mathbf{k}_l(t))\end{aligned}$$
,

$$\partial_{\mathbf{x}} \widetilde{W^\epsilon}(\mathbf{x},\mathbf{k},t) = \sum_{l=1}^{N} \alpha_l(t)\delta'(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t)) \ ,$$

and

$$\partial_{\mathbf{k}} \widetilde{W^\epsilon}(\mathbf{x},\mathbf{k},t) = \sum_{l=1}^{N} \alpha_l(t)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta'(\mathbf{k}-\mathbf{k}_l(t)) \ .$$

The convolution term in (4.2.1) is written as follows

$$\mathcal{Q}^\epsilon(\mathbf{x},\mathbf{k}) *_{\mathbf{k}} \widetilde{W^\epsilon}(\mathbf{x},\mathbf{k},t) = \sum_{l=1}^{N} \mathcal{Q}^\epsilon(\mathbf{x},\mathbf{k}) *_{\mathbf{k}} \left(\alpha_l(t)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t))\right) = \\ = \sum_{l=1}^{N} \alpha_l(t)\mathcal{Q}^\epsilon(\mathbf{x}_l(t),\mathbf{k}-\mathbf{k}_l(t))\delta(\mathbf{x}-\mathbf{x}_l(t))$$

Hence the Wigner equation is transformed to

$$\sum_{l=1}^{N} \dot{\alpha}_l(t)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t)) + \alpha_l(t)\left(\mathbf{k}_l - \dot{\mathbf{x}}_l\right)\delta'(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t)) - \\ - \alpha_l(t)\left(\dot{\mathbf{k}}_l + V'(\mathbf{x}_l)\right)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta'(\mathbf{k}-\mathbf{k}_l(t)) = \sum_{l=1}^{N} \alpha_l(t)\mathcal{Q}^\epsilon(\mathbf{x}_l,\mathbf{k}-\mathbf{k}_l)\delta(\mathbf{x}-\mathbf{x}_l(t)) \tag{4.2.4}$$

Since the particles move along the bicharacteristics, $\mathbf{x}_l(t)$ and $\mathbf{k}_l(t)$), i.e. the solutions of the Hamiltonian system corresponding to the transport operator in the left hand side of (4.2.1),

$$\begin{cases} \dfrac{d\mathbf{x}_l(t)}{dt} = \mathbf{k}_l(t) \\ \dfrac{d\mathbf{k}_l(t)}{dt} = -V'(\mathbf{x}_l(t)), \qquad 1 \le l \le N \\ \mathbf{x}_l(0) = q_l \\ \mathbf{k}_l(t) = p_l \end{cases}$$

Thus, equation (4.2.4) reduces to

$$\sum_{l=1}^{N} \left\{\dot{\alpha}_l(t)\delta(\mathbf{x}-\mathbf{x}_l(t))\delta(\mathbf{k}-\mathbf{k}_l(t))\right\} = \sum_{l=1}^{N} \left\{\alpha_l(t)\mathcal{Q}^\epsilon(\mathbf{x}_l(t),\mathbf{k}-\mathbf{k}_l(t))\delta(\mathbf{x}-\mathbf{x}_l(t))\right\} \tag{4.2.5}$$

Multiplying (4.2.5) by a test function $\phi(\mathbf{x})$ and integrating, we get

$$\sum_{l=1}^{N} \left\{\dot{\alpha}_l(t)\delta(\mathbf{k}-\mathbf{k}_l(t))\right\} = \sum_{l=1}^{N} \left\{\alpha_l(t)\mathcal{Q}^\epsilon(\mathbf{x}_l(t),\mathbf{k}-\mathbf{k}_l(t))\right\} \tag{4.2.6}$$

For $\mathcal{Q}^\epsilon \equiv 0$,which is a case that appears for potentials at most quadratic in $\mathbf{x}$, (4.2.6) becomes

$$\sum_{l=1}^{N} \left\{\dot{\alpha}_l(t)\delta(\mathbf{k}-\mathbf{k}_l(t))\right\} = 0$$

and therefore the weights $\alpha_l(t)$, $1 \le l \le N$ are constant and equal to their initial values α_l^0.

For essential potentials $\mathcal{Q}^\epsilon \not\equiv 0$, we have to solve a system of differential equations for the weights

$$\begin{cases} \dfrac{d\alpha_m(t)}{dt} = \displaystyle\sum_{l=1}^{N} \left\{\alpha_l(t)\mathcal{Q}^\epsilon(\mathbf{x}_l(t),\mathbf{k}_m(t)-\mathbf{k}_l(t))\right\}, \quad m = 1,\ldots,N \\ \alpha_m(0) = \alpha_m^0 \ . \end{cases} \tag{4.2.7}$$

For reducing the size of the numerical computations the set of N particles $\{(\mathbf{x}_l(t), \mathbf{k}_l(t)),\ l = 1, \dots, N\}$ is divided into $J = \frac{N}{M}$ cells with M particles in each cell, for each time t. Then $\mathcal{Q}^\epsilon(\mathbf{x}_l(t), \mathbf{k}_m(t) - \mathbf{k}_l(t))$ is approximated by $\mathcal{Q}^\epsilon(\mathbf{x}_{cj}(t), \mathbf{k}_m(t) - \mathbf{k}_l(t))$ for $l \in cellj, \quad j = 1, \dots, J$, where $\mathbf{x}_{cj}(t)$ is the "mid"-point of $cellj$. Hence instead of solving one system with N equations we solve J independent systems of ODE's with M equations in each system $(j = 1, \dots, J)$

$$
\begin{cases} \dfrac{d\alpha_m(t)}{dt} = \displaystyle\sum_{l \in cellj} \alpha_l(t) \mathcal{Q}^\epsilon(\mathbf{x}_{cj}(t), \mathbf{k}_m(t) - \mathbf{k}_l(t)), \quad m \in cellj \ , \\ \alpha_m(0) = \alpha_m^0 \ . \end{cases} \tag{4.2.8}
$$

Second formulation

In the second formulation, we write the Wigner equation in the form

$$
\begin{cases} \dfrac{dW^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t), t)}{dt} = \mathcal{Z}^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t)) *_\mathbf{k} W^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t), t) \qquad l = 1 \dots N \\ W^\epsilon(\mathbf{x}_l(0), \mathbf{k}_l(0), 0) = W_0^\epsilon(q_l, p_l) \end{cases} \tag{4.2.9}
$$

The first step here is to find an approximation of the convolution term $\mathcal{Z}^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t)) *_\mathbf{k} W^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t), t)$. For this we write

$$
\begin{aligned} \mathcal{Z}^\epsilon(\mathbf{x}, \mathbf{k}) *_\mathbf{k} W^\epsilon(\mathbf{x}, \mathbf{k}, t) &= \int_{\mathbb{R}'_\mathbf{k}} \mathcal{Z}^\epsilon(\mathbf{x}, \mathbf{k} - \mathbf{k}') W^\epsilon(\mathbf{x}, \mathbf{k}', t) d\mathbf{k}' \\ &= \int_{\mathbb{R}'_\mathbf{x}} \int_{\mathbb{R}'_\mathbf{k}} \delta(\mathbf{x} - \mathbf{x}') \mathcal{Z}^\epsilon(\mathbf{x}', \mathbf{k} - \mathbf{k}') W^\epsilon(\mathbf{x}', \mathbf{k}', t) d\mathbf{x}' d\mathbf{k}' \end{aligned} \tag{4.2.10}
$$

and then the delta function is approximated by a cutoff function ζ_η, which gives us

$$
\mathcal{Z}_\eta^\epsilon(\mathbf{x}, \mathbf{k}) *_\mathbf{k} W^\epsilon(\mathbf{x}, \mathbf{k}, t) = \int_{\mathbb{R}'_\mathbf{x}} \int_{\mathbb{R}'_\mathbf{k}} \zeta_\eta(\mathbf{x} - \mathbf{x}') \mathcal{Z}^\epsilon(\mathbf{x}', \mathbf{k} - \mathbf{k}') W^\epsilon(\mathbf{x}', \mathbf{k}', t) d\mathbf{x}' d\mathbf{k}' \ . \tag{4.2.11}
$$

Applying a quadrature rule to $\mathcal{Z}_\eta^\epsilon(\mathbf{x}, \mathbf{k}) *_\mathbf{k} W^\epsilon(\mathbf{x}, \mathbf{k}, t)$ with quadrature points the position and velocity of the particles $\{(\mathbf{x}_j(t), \mathbf{k}_j(t)), \quad j = 1, \dots N\}$, we obtain:

$$
\mathcal{Z}_\eta^\epsilon(\mathbf{x}, \mathbf{k}) *_\mathbf{k} W^\epsilon(\mathbf{x}, \mathbf{k}, t) \approx \sum_j \zeta_\eta(\mathbf{x} - \mathbf{x}_j(t)) \mathcal{Z}^\epsilon(\mathbf{x}_j(t), \mathbf{k} - \mathbf{k}_j(t)) W^\epsilon(\mathbf{x}_j(t), \mathbf{k}_j(t), t) \ . \tag{4.2.12}
$$

From the definition of the particle approximation of W^ϵ, $\widetilde{W^\epsilon}$(4.2.3) we conclude that

$$
\alpha_l(t) \approx W^\epsilon(\mathbf{x}_l(t), \mathbf{k}_l(t), t) \ . \tag{4.2.13}
$$

Therefore the weights $\alpha_l(t)$ must satisfy the system

$$
\begin{cases} \dfrac{d\alpha_l(t)}{dt} = \displaystyle\sum_j \zeta_\eta(\mathbf{x}_l(t) - \mathbf{x}_j(t)) \mathcal{Z}^\epsilon(\mathbf{x}_j(t), \mathbf{k}_l(t) - \mathbf{k}_j(t)) \alpha_j(t), \quad l = 1 \dots N \ , \\ \alpha_l(0) = \alpha_l^0 \ . \end{cases} \tag{4.2.14}
$$

We note that even if $\zeta_\eta(\mathbf{x}) = \delta(\mathbf{x})$, the right hand side of (4.2.14) is not identically zero, in contrast with what happens if we apply this formulation for the Wigner equation (4.2.1).

The convergence of the second formulation is assured only for a "smooth" potential V, which satisfies the conditions:

$$(H1) \quad V \in L^2(\mathbb{R}) \cap L^\infty(\mathbb{R})$$

$$(H2) \quad \int_{\mathbb{R}_v} |v^\alpha||\partial^\beta \widehat{V}(v)|dv < +\infty, \quad \forall(\alpha,\beta), \quad |\alpha+\beta| \le m, m \text{ fixed integer},$$

$(H3)$ there exist C_1, ϵ_1 positive constants, such that

$$|\widehat{V}(v)| \le \frac{c_1}{(1+|v|)^{1+\epsilon_1}}, \quad \widehat{V}(v) \text{ is the Fourier transform of } V.$$

Then, we have the following theorem (compare with Theorem 4.1.2 above).

Theorem 4.2.1

Let

1) ζ is an even compactly supported function such that

$$\int_{\mathbb{R}_x} \zeta(x)dx = 1$$

$$\zeta \in W^{r,1}(\mathbb{R}_x) \text{ for a fixed positive integer } r$$

$$\int_{\mathbb{R}_x} x^\alpha \zeta(x)dx = 0 \text{ ,for all multi-indices } \alpha, \ 1 \le |\alpha| \le r-1$$

2) V satisfies (H1)-(H3) ,

3) the initial data $W_0^\epsilon \in L^2(\mathbb{R}) \cap W^{m,\infty}(\mathbb{R})$. Then,

$$\sup_{t\in[0,T]} \|W^\epsilon(t) - \widetilde{W^\epsilon}(t)\|_{L^\infty(\mathbb{R}^2)} = O(\eta^m + \frac{h^m}{\eta^m}) \ .\blacksquare$$

When V does not satisfy (H1)-(H3), the last tehorem does not hold any more, because we cannot perform a quadrature approximation for the convolution term. If $V \in L^\infty(\mathbb{R})$, then the method that will give an approximate solution to the Wigner equation consists in slightly modifying the original equation by taking a mollified potential $V^\alpha(x) = V(x) *_x \eta^\alpha(x)$. For example, such a mollifier $\eta^\alpha(x)$ is defined by

$$\eta^\alpha(x) = \frac{1}{\alpha}\eta_m(\frac{x}{\alpha}), \quad x \in \mathbb{R} \ ,$$
$$\eta_k = \eta_0 *_x \eta_{k-1}, \qquad 0 < k \le m \ ,$$

with

$$\eta_0(x) = \begin{cases} 1, & \text{if } x \in [-\frac{1}{2}, \frac{1}{2}] \\ 0, & \text{else .} \end{cases}$$

It is proved in [AN] that the solution W_α^ϵ of the Wigner equation with potential V^α converges in $L^2(\mathbb{R}^2)$ to the solution W^ϵ obtained with V, when $\alpha \to 0$. Then, the particle method described above is applied to the regularized equation. The combination of the two approximations yields a convergence in $L^2(\mathbb{R}^2)$ as $\alpha \to 0, \ \eta \to 0, \ \frac{h}{\eta} \to 0$.

4.3 Numerical examples.

In this section we compute the amplitude and the flux of ψ_ϵ, for two characteristic examples, applying the second formulation of the particle method. The first deals with the case of a quadratic potential (harmonic oscillator of quantum mechanics), which is a "non-essential" potential, and the second with the case of a potential barrier which is essentially diffractive. The results derived by the particle method are compared with those produced by the FEM method developed by Akrivis and Dougalis [AD]. It turns out that FEM is accurate and more economical for relatively high frequencies. However, after a certain frequency, depending on time and range, FEM solution seems to produce inaccurate results which can not be improved by diminishing the time step and the grid size. On the other hand, the particle method could be improved by increasing the number of particles, but this becomes very time consuming.

4.3.1 Harmonic oscillator.

We compute the energy density and the flux for the quadratic potential

$$V(x) = \frac{\Omega^2 x^2}{2} , \tag{4.3.1}$$

and Gaussian initial data

$$\begin{aligned} \psi_\epsilon^0(x) &= \alpha_0(x)\exp(\frac{i}{\epsilon}S_0(x)) , \\ \alpha_0(x) &= exp(-\frac{\lambda^2 x^2}{2}), \quad S_0(x) = \frac{\mu^2 x^2}{2} \end{aligned} \tag{4.3.2}$$

where $\Omega,\ \lambda,\ \mu$ are given parameters.

The corresponding Hamiltonian is

$$H(x,k) = \frac{1}{2}k^2 + V(x) = \frac{1}{2}(k^2 + \Omega^2 x^2) , \tag{4.3.3}$$

and the Hamiltonian system is given by

$$\begin{cases} \dfrac{dx}{dt} = \partial_k H = k \\ \dfrac{dk}{dt} = -\partial_x H = -V'(x) = -\Omega^2 x \\ x(0) = q \\ k(0) = p \end{cases} \tag{4.3.4}$$

Solving (4.3.4) we find the bicharacteristics

$$\begin{aligned} x(t) = x(q,p,t) &= qcos(\Omega t) + \frac{p}{\Omega}sin(\Omega t) , \\ k(t) = k(q,p,t) &= -q\Omega sin(\Omega t) + pcos(\Omega t) , \end{aligned} \tag{4.3.5}$$

and solving for the initial point (q,p) we get

$$\begin{aligned} q(x,k,t) &= xcos(\Omega t) - \frac{k}{\Omega}sin(\Omega t) , \\ p(x,k,t) &= x\Omega sin(\Omega t) + kcos(\Omega t) . \end{aligned} \tag{4.3.6}$$

The Wigner transform of the initial data $\psi_\epsilon^0(x)$ is

(4.3.7)

$$W_0^\epsilon(q,p) = \frac{1}{\pi\epsilon}\int_{-\infty}^{+\infty} exp(-i\frac{2p}{\epsilon}\sigma)\psi_\epsilon^0(q+\sigma)\overline{\psi_\epsilon^0}(q-\sigma)d\sigma =$$
$$= \frac{1}{\pi\epsilon}\int_{-\infty}^{+\infty} exp(-i\frac{2p}{\epsilon}\sigma)exp[-\frac{\lambda^2}{2}[(q+\sigma)^2+(q-\sigma)^2]]exp[i\frac{\mu^2}{2\epsilon}[(q+\sigma)^2-(q-\sigma)^2]]d\sigma =$$
$$= \frac{1}{\pi\epsilon}e^{-\lambda^2q^2}\int_{-\infty}^{+\infty} e^{-\lambda^2\sigma^2}exp[-i\frac{2}{\epsilon}(p-\mu^2q)\sigma]d\sigma = \frac{1}{\sqrt{\pi}}\frac{e^{-\lambda^2q^2}}{\lambda\epsilon}exp\left(-\frac{(p-\mu^2q)^2}{(\lambda\epsilon)^2}\right) .$$

Hence the solution of the Wigner equation, which here coincides with the limit Wigner equation, is given by

$$W^\epsilon(x,k,t) = W_0^\epsilon\left(q(x,k,t),p(x,k,t)\right) = W_0^\epsilon\left(xcos(\Omega t)-\frac{k}{\Omega}sin(\Omega t), x\Omega sin(\Omega t)+kcos(\Omega t)\right) .$$

Then, the energy density is

$$|\psi_\epsilon(x,t)|^2 = \int_{-\infty}^{+\infty} W^\epsilon(x,k,t)dk = \frac{1}{\sqrt{\pi}}\frac{1}{\lambda\epsilon}\int_{-\infty}^{+\infty} e^{-(A+Bk)^2}e^{-(\Gamma+\Delta k)^2}dk =$$
$$= \frac{1}{\lambda\epsilon\sqrt{B^2+\Delta^2}}exp\left[-\left(\frac{x}{\epsilon}\right)^2\frac{1}{B^2+\Delta^2}\right] . \tag{4.3.8}$$

where

$$A = \lambda xcos(\Omega t) , \qquad B = -\frac{\lambda sin(\Omega t)}{\Omega}$$
$$\Gamma = \Gamma(\epsilon) = \frac{1}{\lambda\epsilon}\left(\Omega xsin(\Omega t)-\mu^2xcos(\Omega t)\right) \tag{4.3.9}$$
$$\Delta = \Delta(\epsilon) = \frac{1}{\lambda\epsilon}\left(cos(\Omega t)+\mu^2\frac{sin(\Omega t)}{\Omega}\right)$$

Moreover, the energy flux is given by

$$\mathcal{F}(x,t) = |\psi_\epsilon(x,t)|^2\phi_\epsilon'(x,t) = \int_{-\infty}^{+\infty} kW^\epsilon(x,k,t)dk =$$
$$= -\frac{AB+\Gamma\Delta}{(B^2+\Delta^2)^{\frac{3}{2}}}exp\left[-\left(\frac{x}{\epsilon}\right)^2\frac{1}{B^2+\Delta^2}\right] = \tag{4.3.10}$$
$$= -|\psi_\epsilon(x,t)|^2\frac{AB+\Gamma\Delta}{B^2+\Delta^2} ,$$

and therefore the derivative of the phase is

$$\phi_\epsilon'(x,t) = \frac{AB+\Gamma\Delta}{B^2+\Delta^2} . \tag{4.3.11}$$

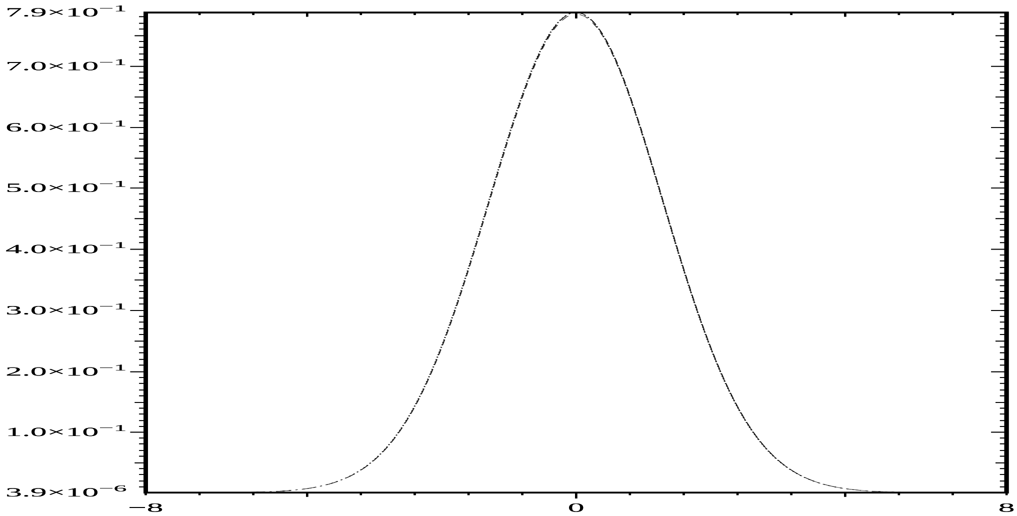
We note that $|\psi_\epsilon(x,t)|$ remains finite even at the focal points

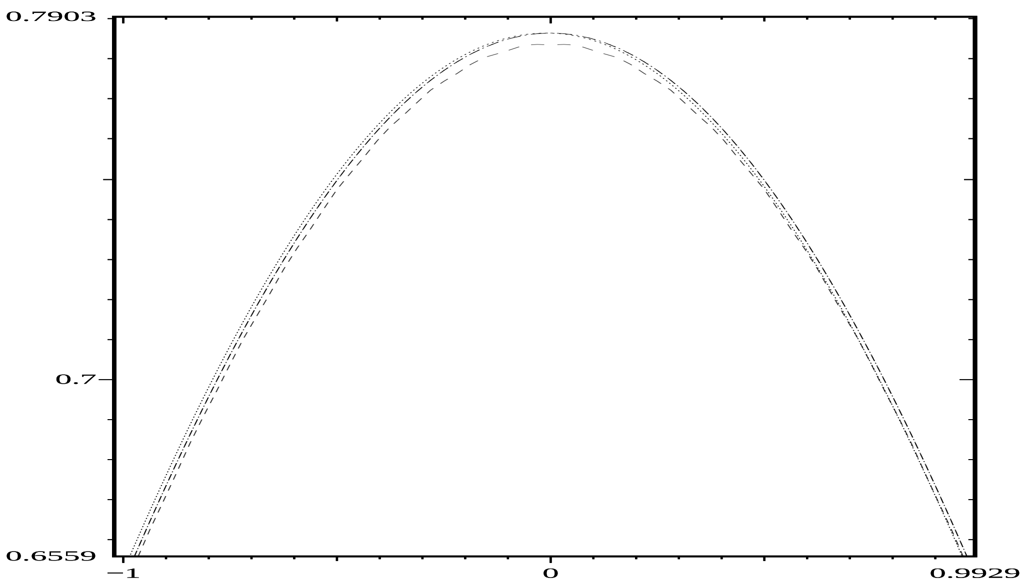
$$x = 0 , \qquad t_m = (m-1/4)\pi/\Omega , m = 1,2,\ldots ,$$

where WKB predicts infinite amplitudes.

In Figures 1-7 we show the variation of $\mid \psi_\epsilon \mid$ and $\mathcal{F}$ with respect to x, for $t = 1, 5$ and $\epsilon = 1, 0.1, 0.01$. We observe that for $t = 1$ the particle and FEM solutions coincide with the analytical solution, the amplitudes showing a better agreement compared with the phases. The same behavior is observed for $t = 5$ (longer range). However, for ϵ smaller than $\epsilon = 0.001$, both numerical solutions deviate significantly from the analytical one. The FEM solution can not be improved by diminishing the time step and the grid size. But on the other hand we cannot significantly improve the particle solution, since we should increase very much the number of particles.

The numerical results for the particle method were smoothed in order to be able to compare with the analytic solution or with the FEM solution. These smoothed results are shown in the Figures 3a-3c,4a,4b. For the smoothing we applied we applied a Savitzky-Golay smoothing filter (subroutine: savgol.f, from Numerical Recipies software library).

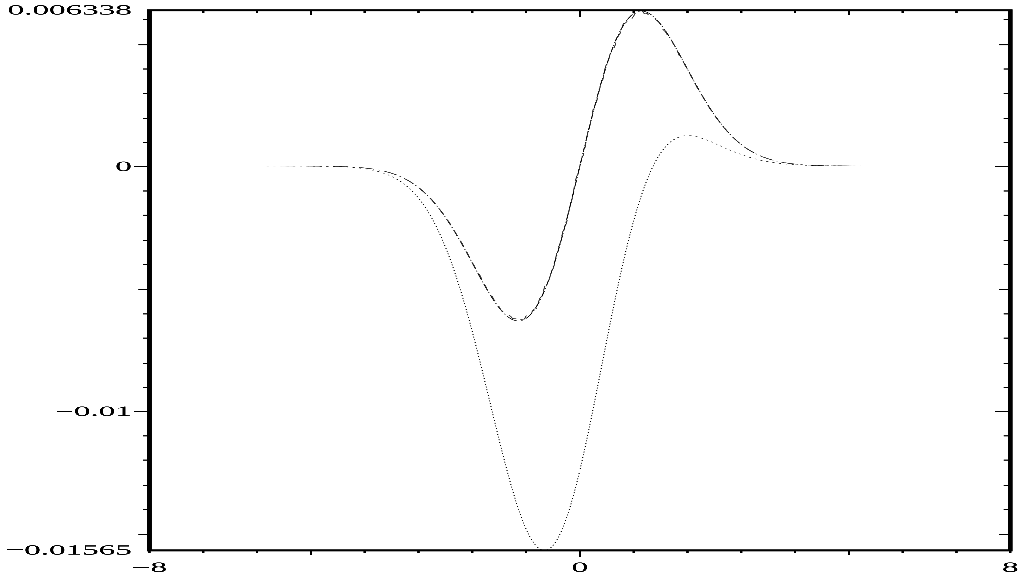


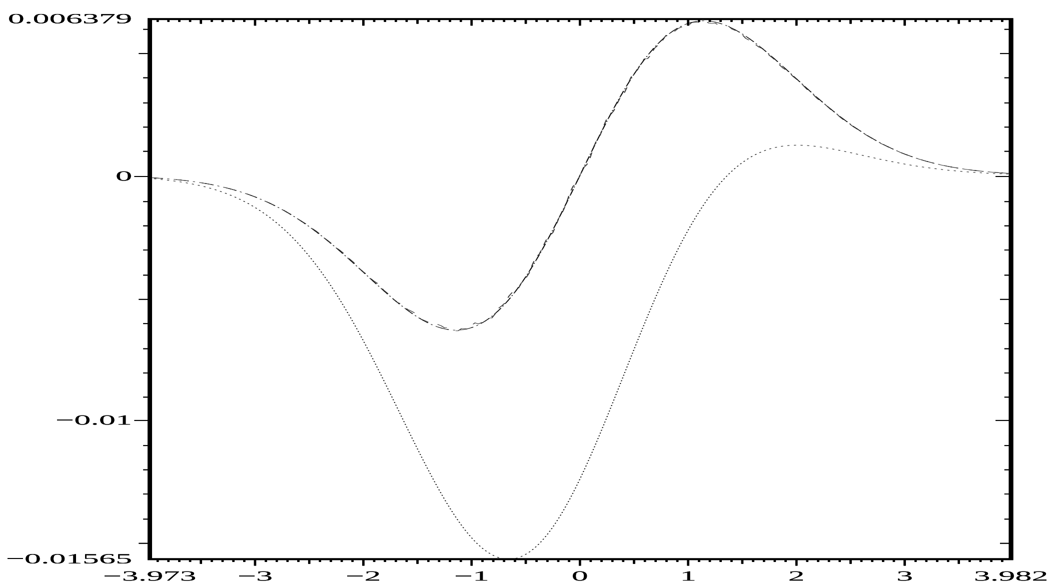


$Figures\ 1a : |\psi_\epsilon(x, t = 1)|^2, \epsilon = 1\ vs.\ x$

$Particle(\#P = 90000\ time = 39.41),\ FEM(\ time = 14.09)$

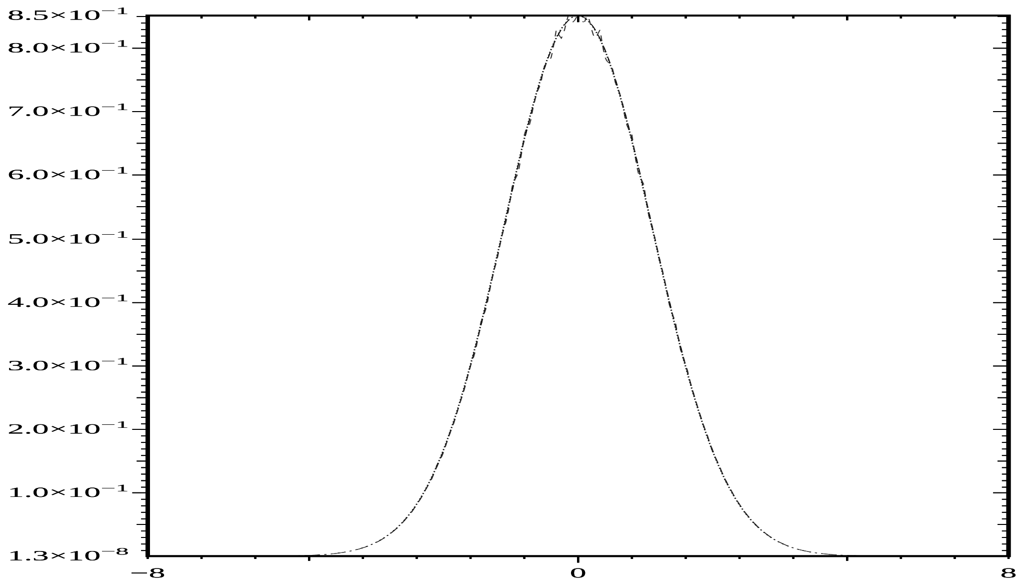
$(- \cdot - \cdot -\ Analytical\ Solution, - - - Wigner\ Solution,\ \cdots\ FEM\ Solution)$

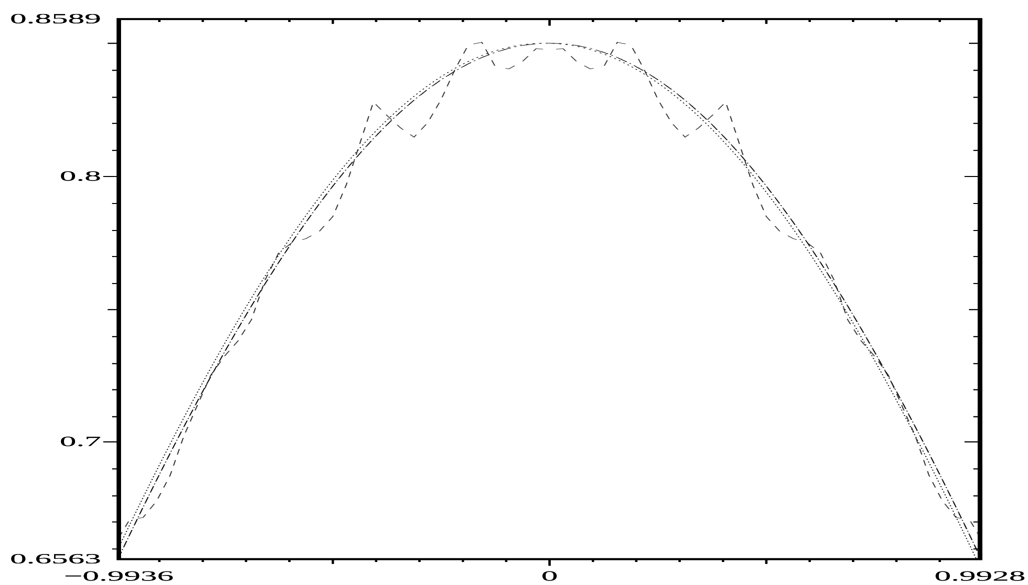




$Figures\ 1b : \mathcal{F}(x,t=1), \epsilon = 1\ vs.\ x$

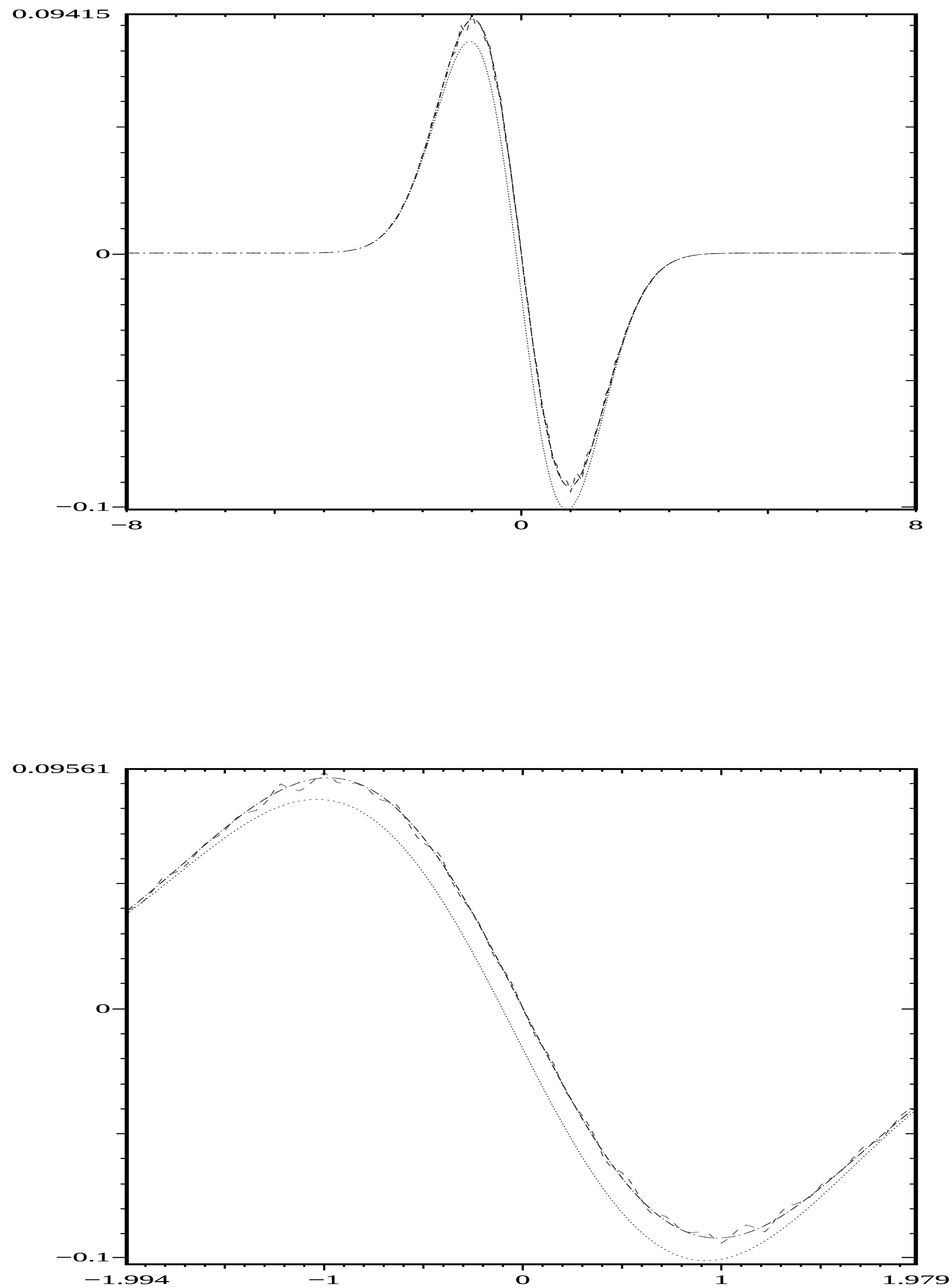
$Particle(\#P = 90000\ time = 39.41),\ \ FEM(\ time = 14.09)$





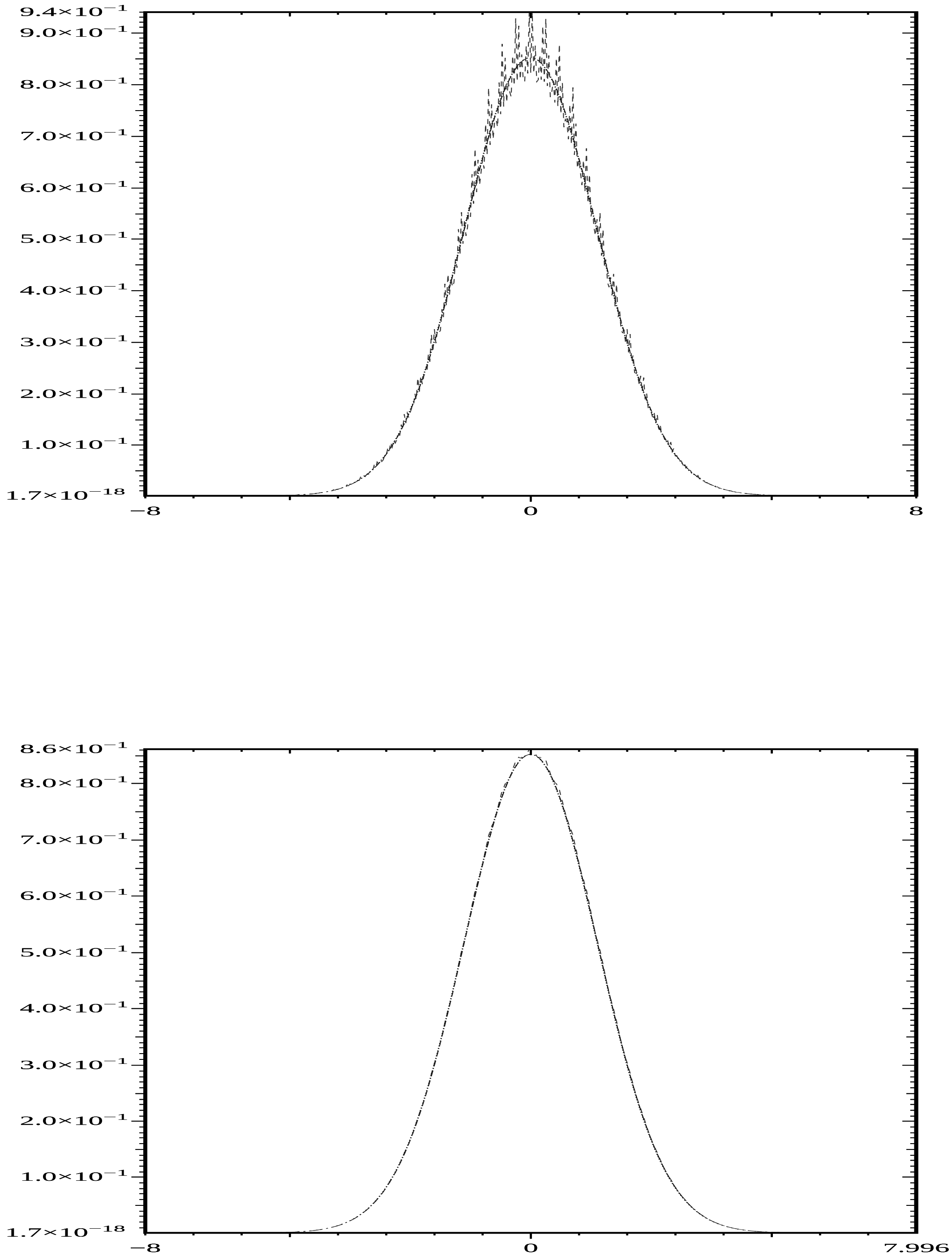
$Figures\ 2a : |\psi_\epsilon(x,t=1)|^2, \epsilon = 0.1\ vs.\ x$

$Particle(\#P = 90000\ time = 39.41),\ FEM(\ time = 14.15)$



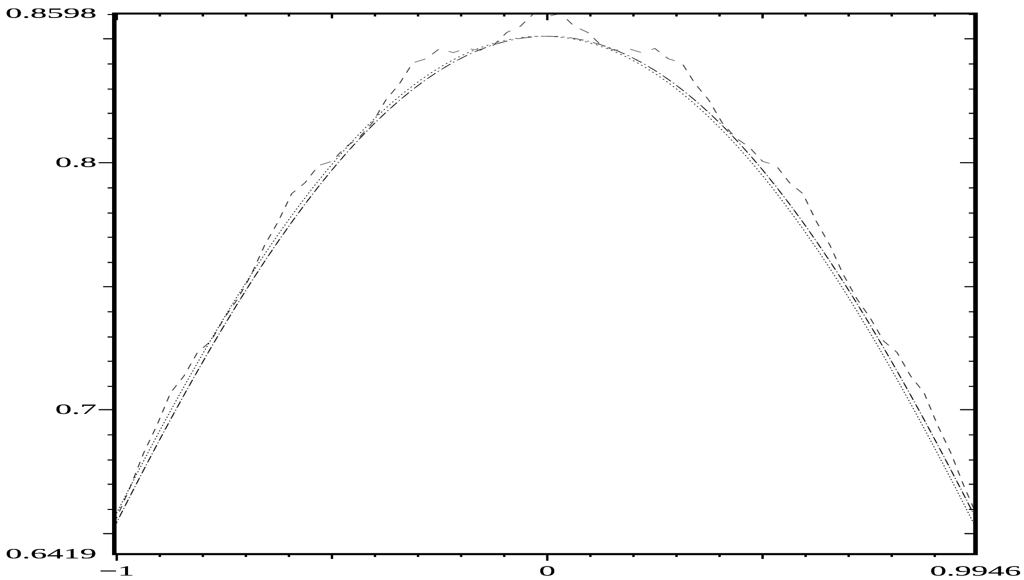
$Figures\ 2b : \mathcal{F}(x, t = 1), \epsilon = 0.1\ vs.\ x$

$Particle(\#P = 90000\ time = 39.41),\ \ FEM(\ time = 14.15)$



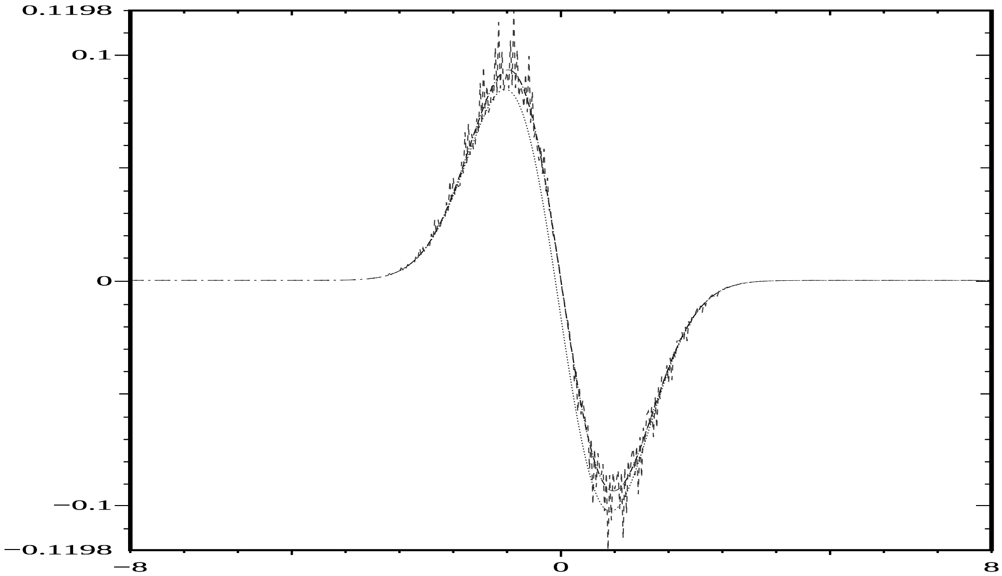
$$Figures\ 3a : |\psi_\epsilon(x, t = 1)|^2,\ \epsilon = 0.01,\ vs.\ x$$

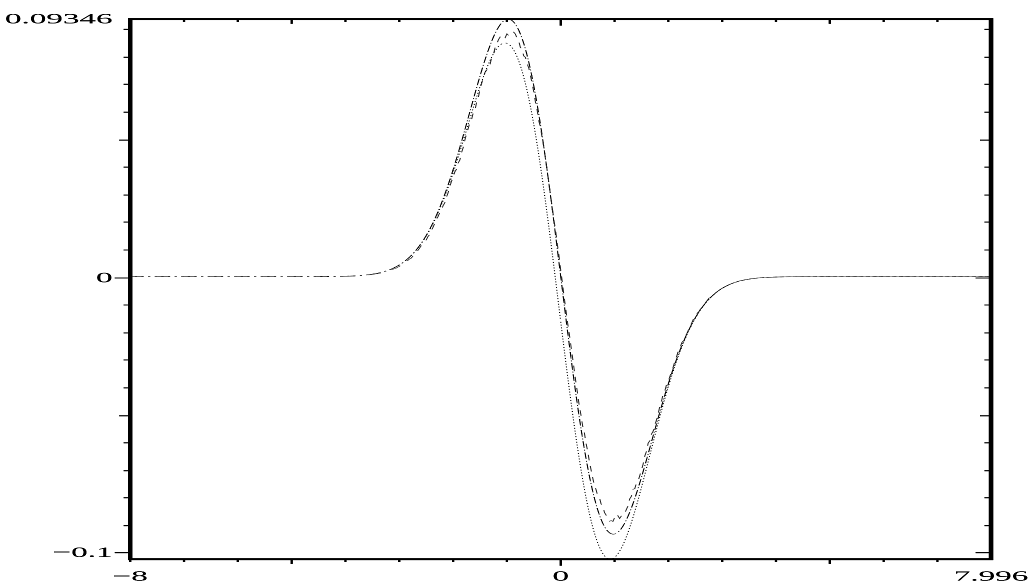
$$Particle : \#P = 1210000\ time = 547.26\ FEM :\ time = 13.94$$



$Figures\ 3b : |\psi_\epsilon(x, t = 1)|^2,\ \epsilon = 0.01,\ vs.\ x$

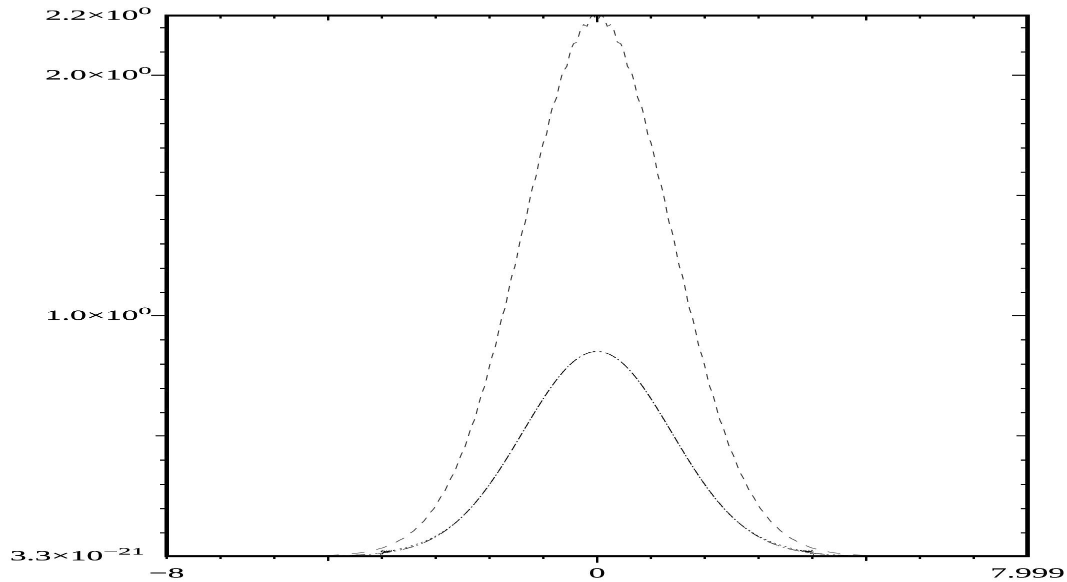
$Particle(\#P = 1210000\ time = 547.26),\ FEM(\ time = 13.94)$

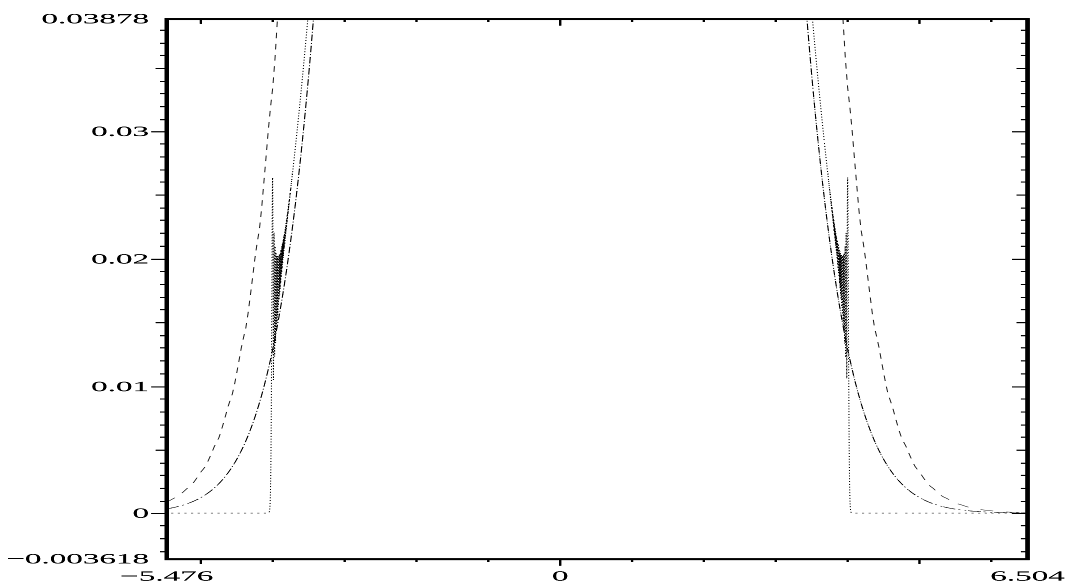




$Figures\ 3c : \mathcal{F}(x, t = 1)\ , \epsilon = 0.01\ vs.\ x$

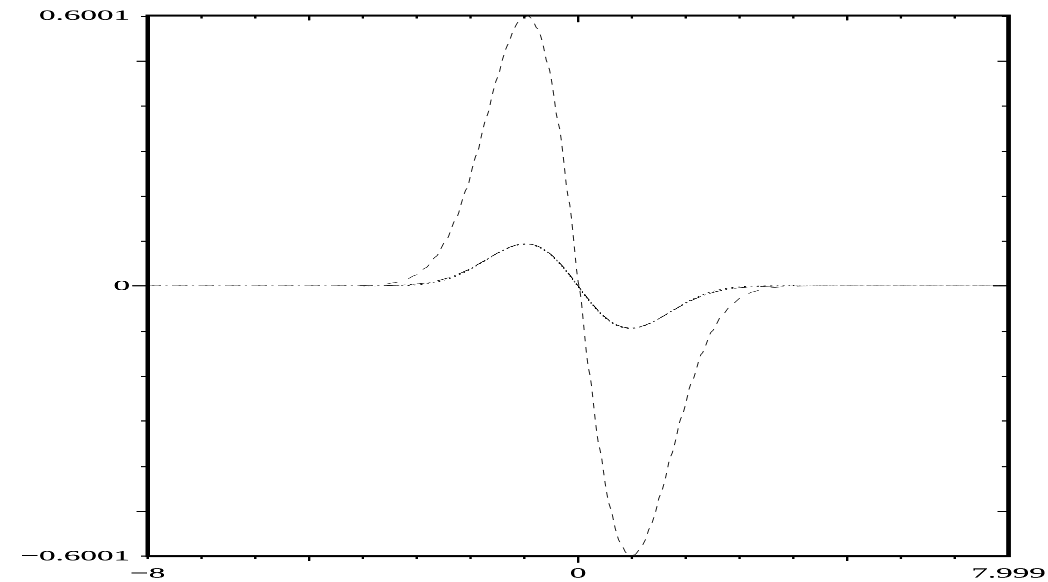
$Particle(\#P = 1210000\ time = 547.26),\ \ FEM(\ time = 13.94)$

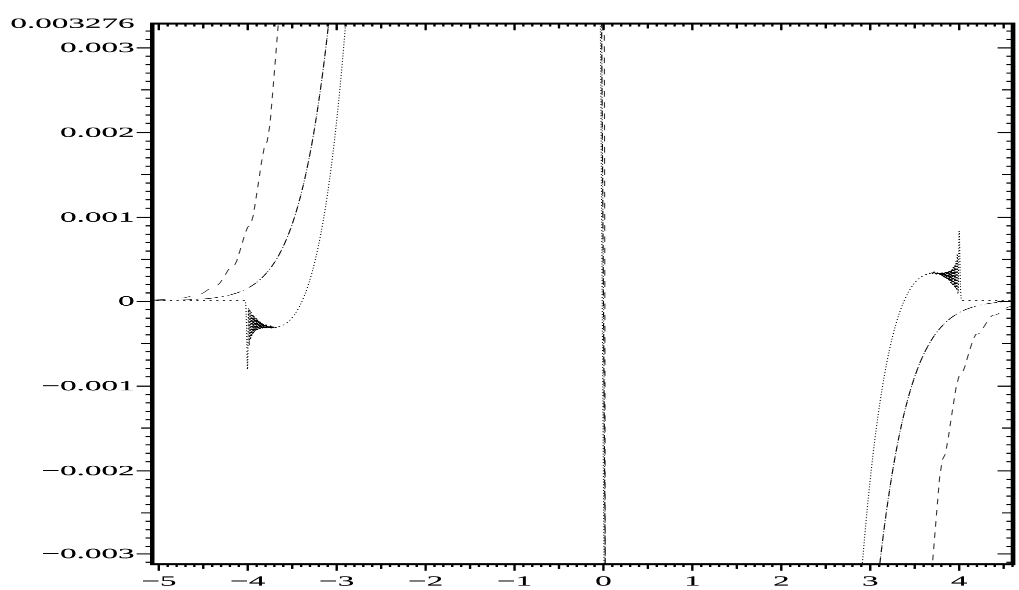




$Figures\ 4a : |\psi_\epsilon(x,t=1)|^2\ , \epsilon = 0.001\ vs.\ x$

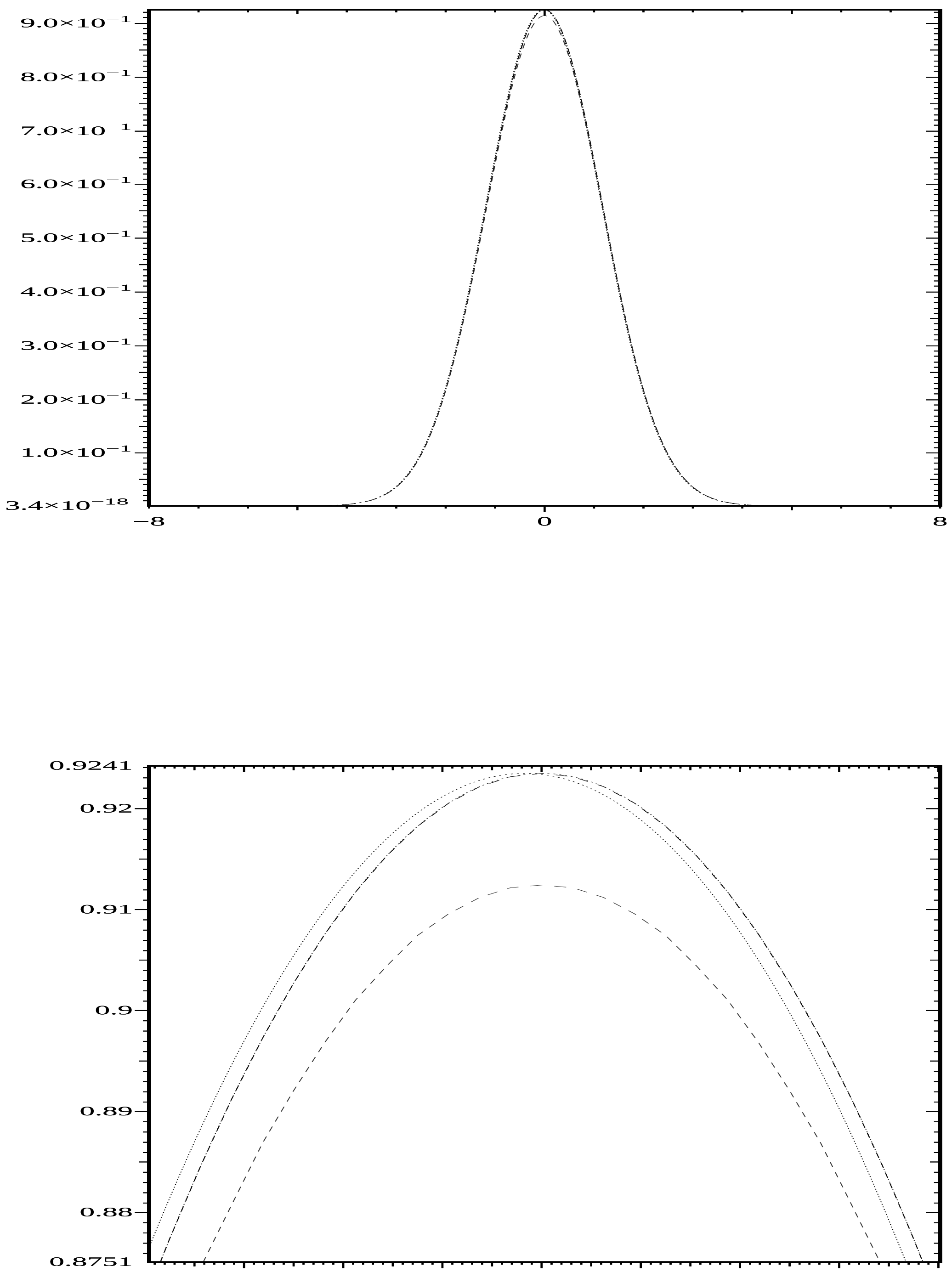
$Particle(\#P = 1690000\ time = 764.17),\ \ FEM(\ time = 251.11)$





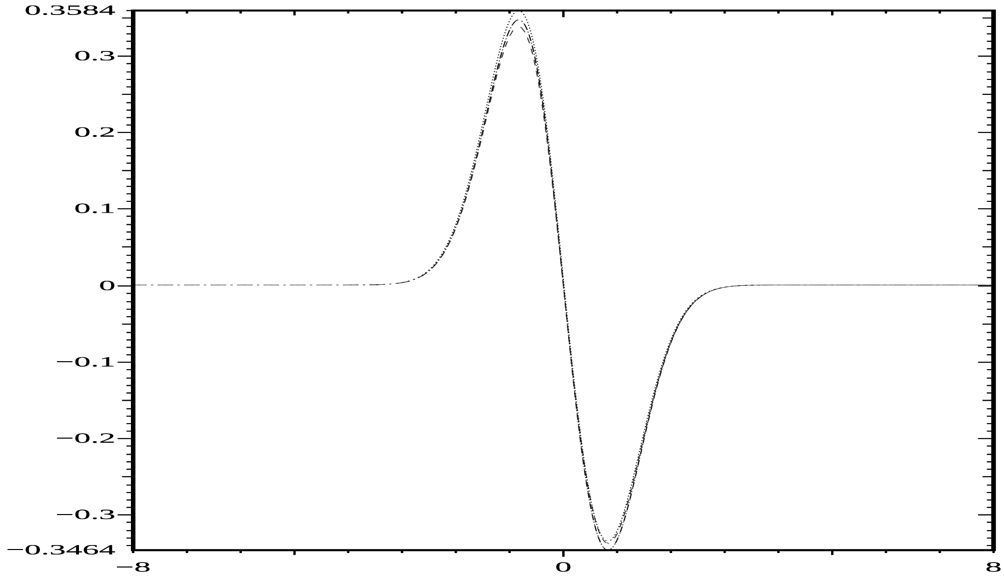
$Figures\ 4b : \mathcal{F}(x, t = 1)\ , \epsilon = 0.01\ vs.\ x$

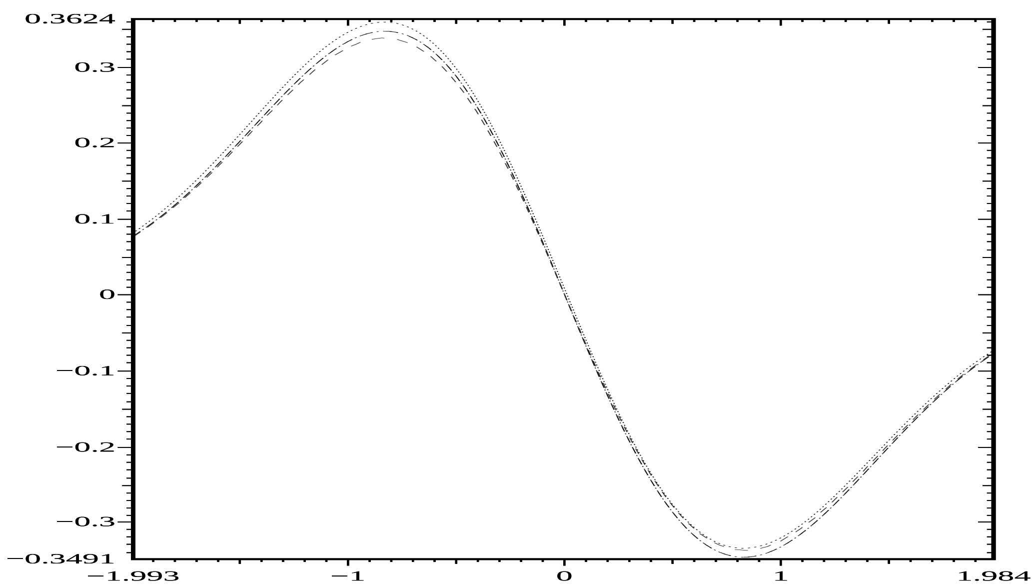
$Particle(\#P = 1690000\ time = 764.17),\ \ FEM(\ time = 251.11)$



$Figures\ 5a : |\psi_\epsilon(x, t = 5)|^2,\ \epsilon = 1\ vs.\ x$

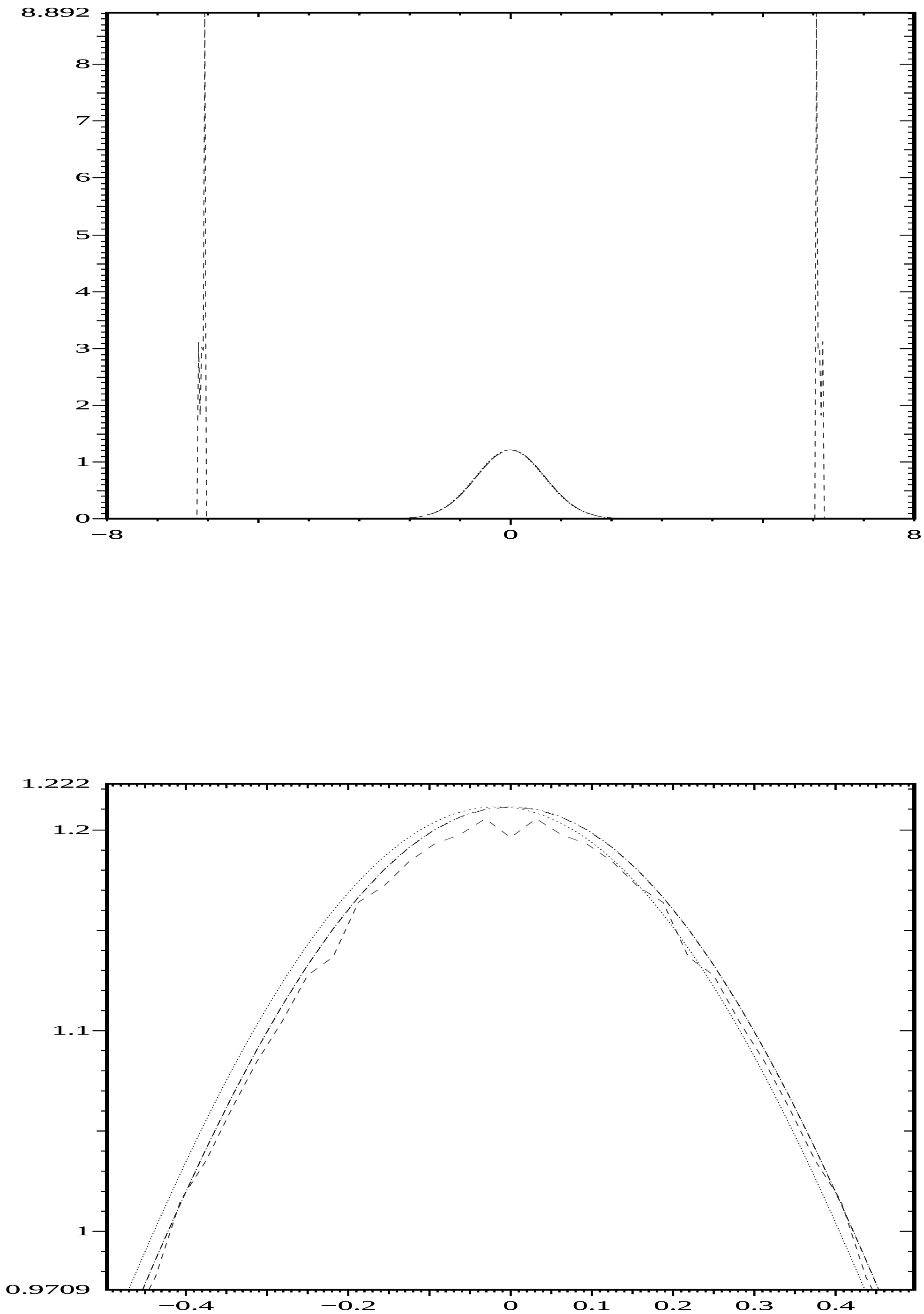
$Particle(\#P = 10000\ time = 17.76),\ FEM(\ time = 13.87)$





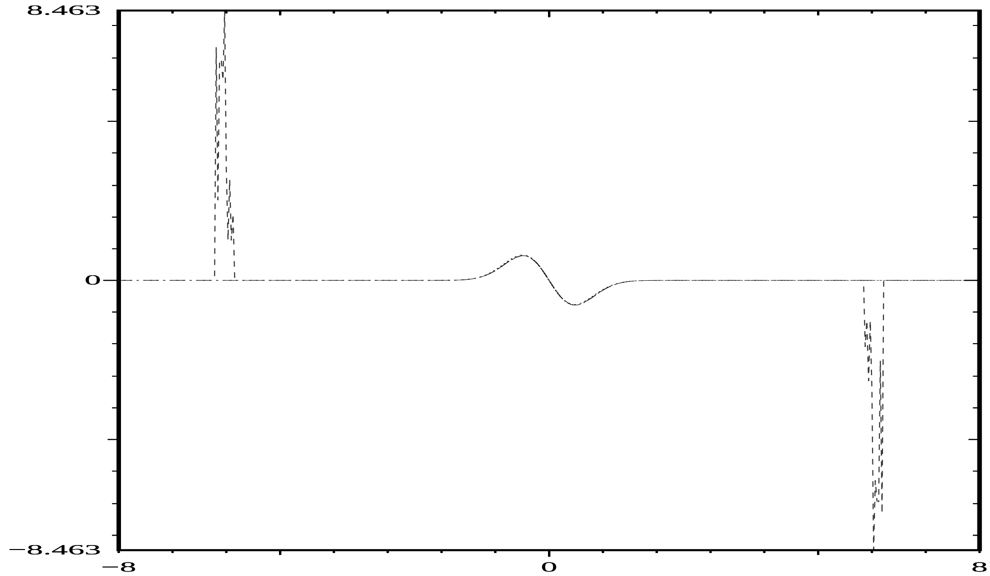
$Figures\ 5b : \mathcal{F}(x, t = 5),\ \epsilon = 1\ vs.\ x$

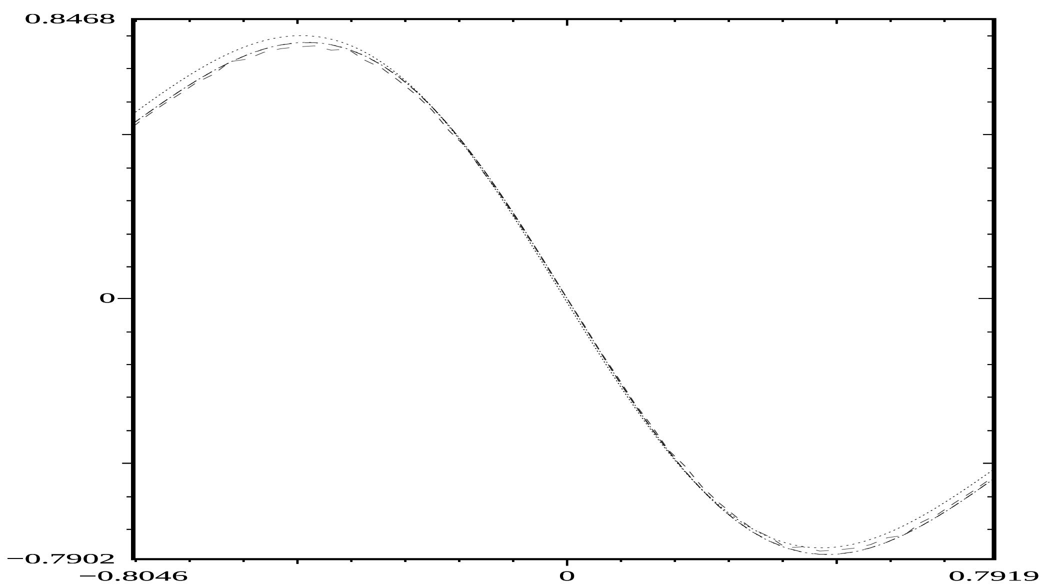
$Particle(\#P = 10000\ time = 17.76),\ FEM(\ time = 13.87)$



$Figures\ 6a : |\psi_\epsilon(x, t = 5)|^2,\ \epsilon = 0.1\ vs.\ x$

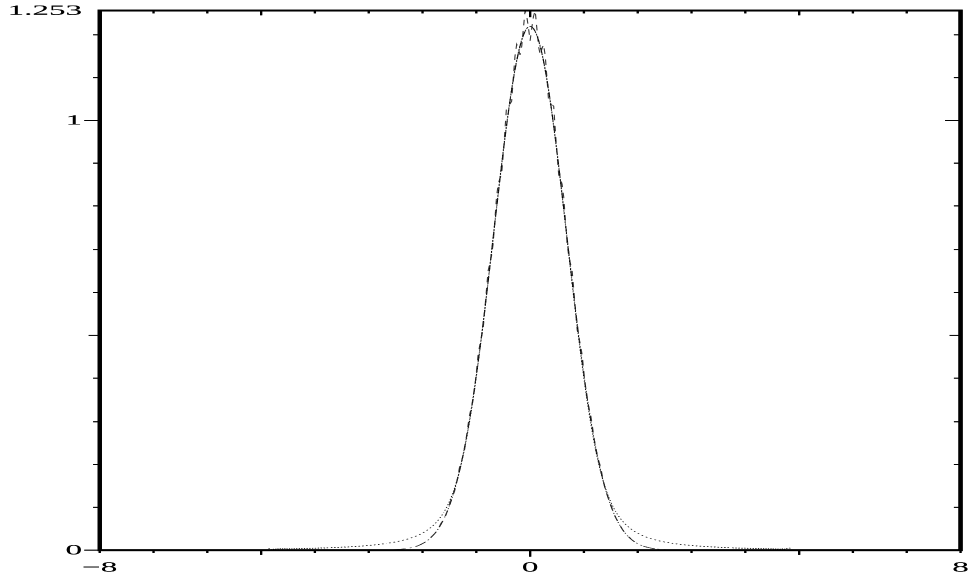
$Particle(\#P = 40000\ time = 70.78),\ FEM(\ time = 14.01)$

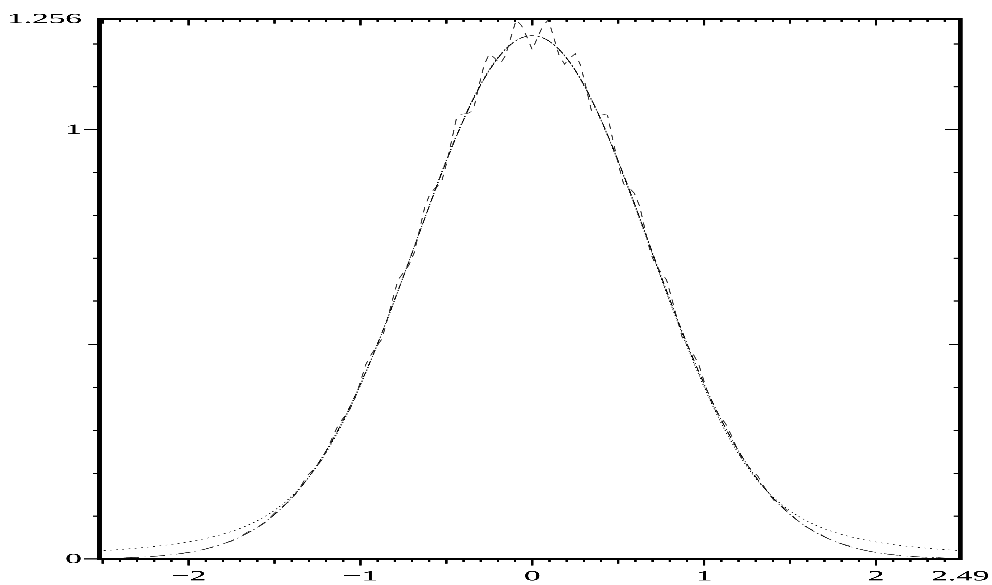




$Figures\ 6b : \mathcal{F}(x, t = 5),\ \epsilon = 0.1\ vs.\ x$

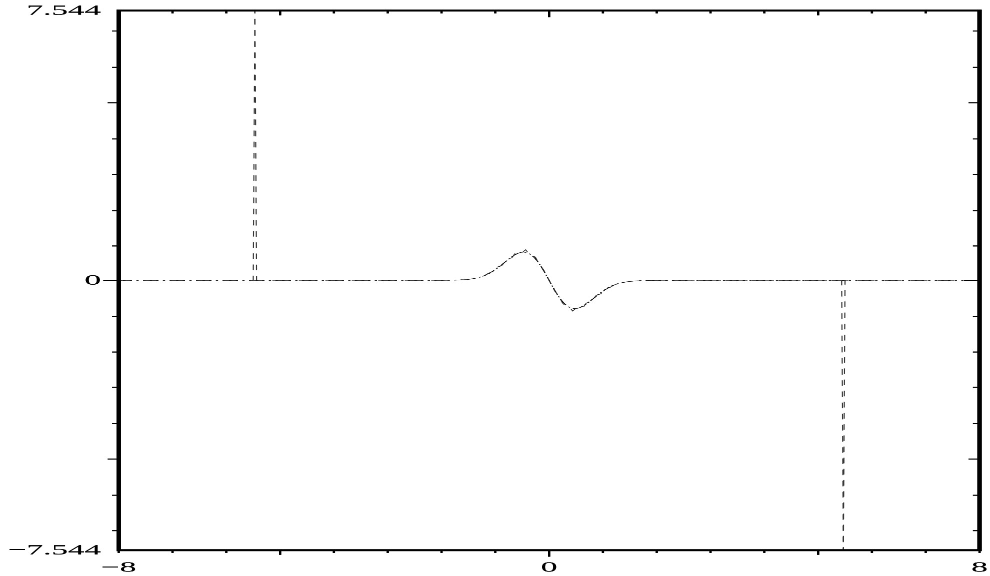
$Particle(\#P = 40000\ time = 70.78),\ FEM(\ time = 14.01)$

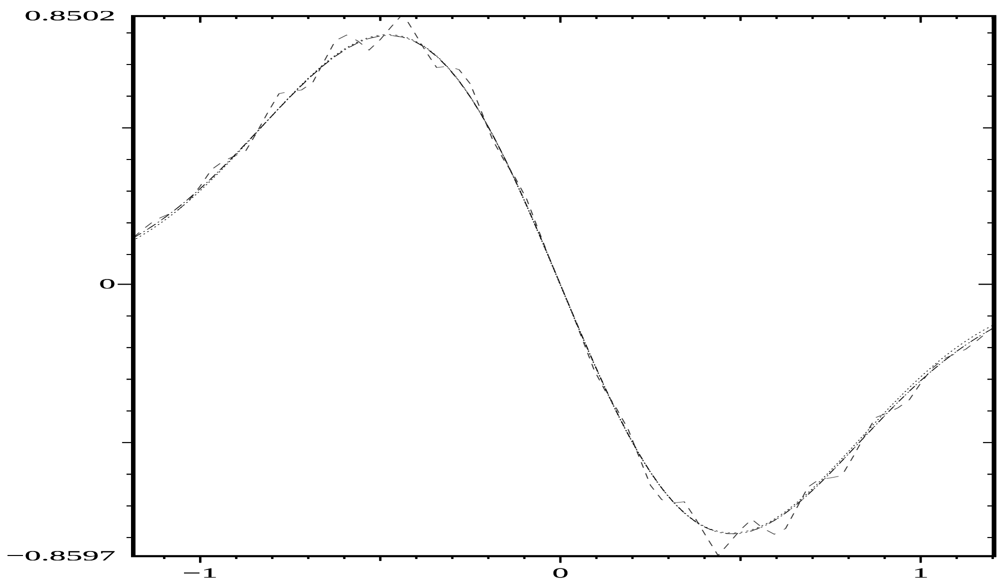




$$Figures\ 7a : |\psi_\epsilon(x,t=5)|^2,\ \epsilon = 0.01\ vs.\ x$$

$$Particle(\#P = 1210000\ time = 2193.49),\ \ FEM(\ time = 251.04)$$





$Figures\ 7b : \mathcal{F}(x, t = 5),\ \epsilon = 0.01\ vs.\ x$

$Particle(\#P = 1210000\ time = 2193.49),\ FEM(\ time = 251.04)$

4.3.2 Potential barrier.

We consider now the Schrödinger equation with potential

$$V(x) = \begin{cases} 1, & x \in [-b, b] \\ 0, & elsewhere \end{cases} , \tag{4.3.12}$$

and with the same initial data as in the previous example for the harmonic oscillator. We want again to compute the energy density and the energy flux.

Recall that the Wigner equation is

$$\partial_t W^\epsilon(x,k,t) + k\partial_x W^\epsilon(x,k,t) = \mathcal{Z}^\epsilon(x,k) *_k W^\epsilon(x,k,t) ,$$

where $\mathcal{Z}^\epsilon$ is given by (3.2.4).

The potential $V(x)$ does not satisfy the Hypothesis 1 of Section 4.2, so we cannot apply the second formulation of the particle method directly, but we need to use, instead of $V(x)$, a mollified potential

$$V_\alpha(x) = \eta^\alpha(x) * V(x) , \tag{4.3.13}$$

where η^α is an appropriate mollifier, and to solve the equation

$$\partial_t W_\alpha^\epsilon(x,k,t) + k\partial_x W_\alpha^\epsilon(x,k,t) = Z_\alpha^\epsilon(x,k) *_k W_\alpha^\epsilon(x,k,t) , \tag{4.3.14}$$

with

$$Z_\alpha^\epsilon(x,k) = \frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V_\alpha(x+\frac{\epsilon}{2}y) - V_\alpha(x-\frac{\epsilon}{2}y)\right)dy . \tag{4.3.15}$$

Note that $\mathcal{Z}^\epsilon$ can be expresses in terms of the Fourier transform of V_α as follows

$$Z_\alpha^\epsilon(x,k) = \frac{4}{\epsilon^2} Im\left[e^{i\frac{2k}{\epsilon}x}\widehat{V}_\alpha(\frac{2k}{\epsilon})\right] . \tag{4.3.16}$$

In fact, we have

$$\begin{aligned}
Z_\alpha^\epsilon(x,k) =& \frac{1}{i\epsilon}\frac{1}{2\pi}\int_{\mathbb{R}} e^{-iky}\left(V_\alpha(x+\frac{\epsilon}{2}y) - V_\alpha(x-\frac{\epsilon}{2}y)\right)dy \\
=& \frac{1}{2\pi}\frac{1}{i\epsilon}\frac{2}{\epsilon}\int_{\mathbb{R}} e^{-i\frac{2k}{\epsilon}y}\left(V_\alpha(x+y) - V_\alpha(x-y)\right)dy \\
=& \frac{1}{i\pi\epsilon^2}\left[\int_{\mathbb{R}} exp(-i\frac{2k}{\epsilon}(z-x))V_\alpha(z)dz - \int_{\mathbb{R}} exp(-i\frac{2k}{\epsilon}(x-z))V_\alpha(z)dz\right] \\
=& 2\pi\frac{1}{i\pi\epsilon^2}\left[e^{i\frac{2k}{\epsilon}x}\frac{1}{2\pi}\int_{\mathbb{R}} e^{-i\frac{2k}{\epsilon}z}V_\alpha(z)dz - e^{-i\frac{2k}{\epsilon}x}\frac{1}{2\pi}\int_{\mathbb{R}} e^{i\frac{2k}{\epsilon}z}V_\alpha(z)dz\right] \\
=& \frac{2}{i\epsilon^2}\left[e^{i\frac{2k}{\epsilon}x}\widehat{V}_\alpha(\frac{2k}{\epsilon}) - \overline{e^{i\frac{2k}{\epsilon}x}\widehat{V}_\alpha(\frac{2k}{\epsilon})}\right] = \frac{4}{\epsilon^2} Im\left[e^{i\frac{2k}{\epsilon}x}\widehat{V}_\alpha(\frac{2k}{\epsilon})\right] .
\end{aligned}$$

In the sequel, we use the mollifier

$$\eta^\alpha(x) = \frac{1}{\alpha\sqrt{\pi}} exp(-\frac{x^2}{\alpha^2}) . \tag{4.3.17}$$

Then, we have

$$\widehat{V}_\alpha(\xi) = 2\pi \widehat{V}(\xi)\widehat{\eta}^\alpha(\xi) \ , \tag{4.3.18}$$

where

$$\widehat{V}(\xi) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-i\xi x}V(x)dx = \frac{1}{\pi}\frac{\sin(\xi b)}{\xi} \ , \tag{4.3.19}$$

and

$$\widehat{\eta}^\alpha(\xi) = \frac{1}{2\pi}e^{-\alpha^2\frac{\xi^2}{4}} \ . \tag{3.3.20}$$

Thus

$$\widehat{V}_\alpha(\xi) = \frac{1}{\pi}e^{-\alpha^2\frac{\xi^2}{4}}\frac{\sin(\xi b)}{\xi} \ , \tag{4.3.21}$$

and

$$Z_\alpha^\epsilon(x,k) = \frac{2}{\pi\epsilon k}\sin\left(\frac{2k}{\epsilon}x\right)\sin\left(\frac{2k}{\epsilon}b\right) exp\left(-\alpha^2\frac{k^2}{\epsilon^2}\right) \ . \tag{4.3.22}$$

The Hamiltonian system for the second particle formulation ($k = \text{const.}$) is given by

$$\left.\begin{aligned} \frac{dx}{dt} &= k, \quad x(0) = q \\ \frac{dk}{dt} &= 0, \quad k(0) = p \end{aligned}\right\} \ , \tag{4.3.23}$$

and the bicharacteristics are

$$x(t) = pt + q, \quad k(t) = p \ . \tag{4.3.24}$$

For the application of the particle method, we use again a uniform distribution of initial particles $(q_l, p_l), \quad l = 1, \dots, N$. Their position after time t is simply given by

$$x_l(t) = p_l t + q_l, \quad k_l(t) = p_l, \quad l = 1, \dots, N \ , \quad t > 0 \ , \tag{4.3.25}$$

and the weights $\alpha_l(t)$ solve the system

$$\frac{d\alpha_l}{dt}(t) = \sum_{m=1}^{N} \alpha_m(t) Z_\alpha^\epsilon(x_m(t), k_l(t) - k_m(t)), \quad l = 1, \dots, N \ . \tag{4.3.26}$$

Finally, the corresponding limit Wigner equation

$$\partial_t W_\alpha^\epsilon(x,k,t) + k\partial_x W_\alpha^\epsilon(x,k,t) - V_\alpha^{'}(x)\partial_k W_\alpha^\epsilon(x,k,t) = 0 \ , \tag{4.3.27}$$

can be written explicitly. In fact, we have

$$\begin{aligned} V_\alpha(x) &= \int_{\mathbb{R}} e^{i\xi x}\widehat{V}_\alpha(\xi)d\xi == \frac{1}{\pi}\int_{\mathbb{R}} e^{i\xi x}e^{-\alpha^2\frac{\xi^2}{4}}\frac{\sin(\xi b)}{\xi}d\xi \\ &= \frac{1}{\pi}\left(\int_{\mathbb{R}} e^{-\alpha^2\frac{\xi^2}{4}}\frac{\cos(\xi x)\sin(\xi b)}{\xi}d\xi + \int_{\mathbb{R}} e^{-\alpha^2\frac{\xi^2}{4}}\frac{\sin(\xi x)\sin(\xi b)}{\xi}d\xi\right) \\ &= \frac{1}{\pi}\left(I_1 + I_2\right) \ . \end{aligned}$$

But, $I_2 = 0$ since the integrand is an odd function of ξ, and

$$\begin{aligned} I_1 &= 2\int_0^\infty e^{-\alpha^2\frac{\xi^2}{4}}\frac{\cos(\xi x)\sin(\xi b)}{\xi}d\xi = \int_0^\infty \frac{\sin[\xi(b+x)] + \sin[\xi(b-x)]}{\xi}d\xi \\ &= \int_0^\infty \frac{\sin[\xi(b+x)]}{\xi}d\xi + \int_0^\infty \frac{\sin[\xi(b-x)]}{\xi}d\xi = \frac{\pi}{2}\left(\Phi\left(\frac{b+x}{\alpha}\right) + \Phi\left(\frac{b-x}{\alpha}\right)\right) \end{aligned}$$

where Φ is the error function

$$\Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt \ ..$$

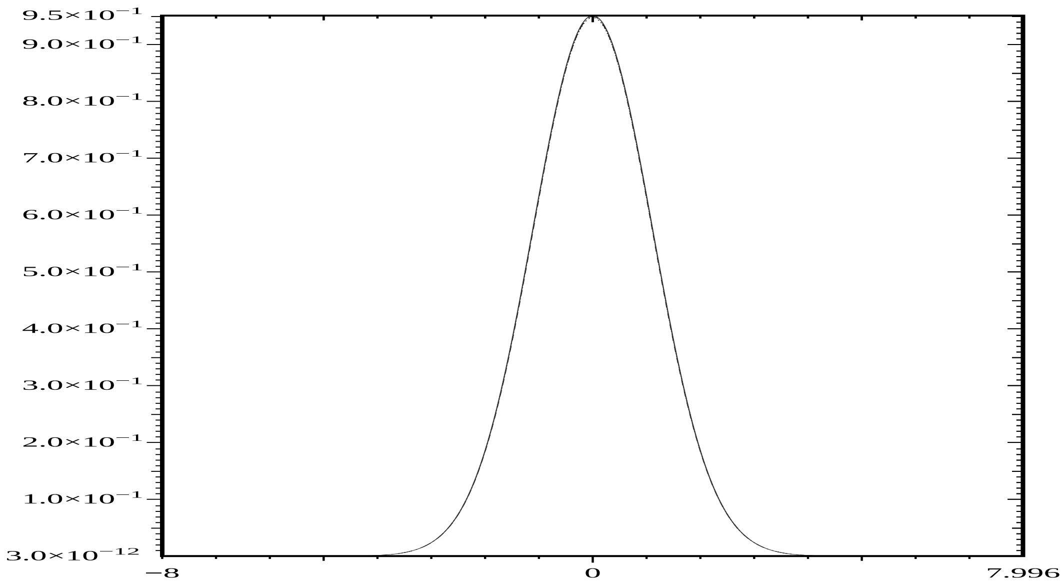
Thus

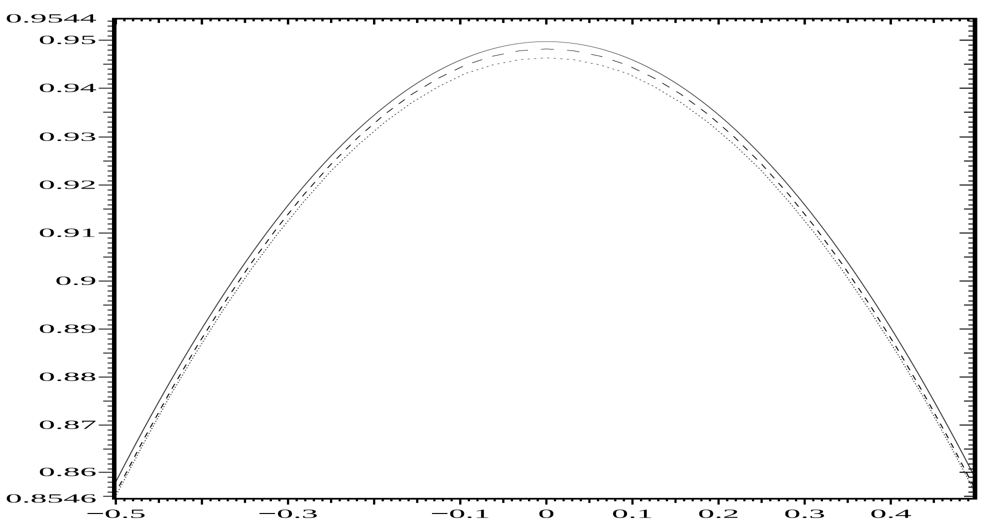
$$V_\alpha(x) = \frac{1}{\pi}I_1 = \frac{1}{2}\Phi\left(\frac{b+x}{\alpha}\right) + \frac{1}{2}\Phi\left(\frac{b-x}{\alpha}\right) \ ,$$

and

$$\begin{aligned} V_\alpha^{'}(x) =& \frac{1}{2\alpha}\left[\Phi^{'}\left(\frac{b+x}{\alpha}\right) - \Phi^{'}\left(\frac{b-x}{\alpha}\right)\right] \\ =& \frac{1}{2\alpha}\frac{2}{\sqrt{\pi}}\left\{exp\left[-(\frac{b+x}{\alpha})^2\right] - exp\left[-(\frac{b-x}{\alpha})^2\right]\right\} \\ =& \frac{1}{\alpha\sqrt{\pi}}\left\{exp\left[-\left(\frac{b+x}{\alpha}\right)^2\right] - exp\left[-\left(\frac{b-x}{\alpha}\right)^2\right]\right\}. \end{aligned} \tag{4.3.28}$$

In the Figures 8-19, we show again the variation of the amplitude $\mid \psi_\epsilon \mid$ and the flux $\mathcal{F}$ with respect to x, for $t = 0.1, 0.8, 1, 2$ and $\epsilon = 1, 0.1, 0.01, 0.001$. In the numerical computation we use $\zeta_\eta(x) \equiv 1$(cf. Section 4.2). Now an analytical solution is not available. So we compare the particle and FEM solutions, and also with the particle solution of the limit Wigner equation. Smoothed results of the particle code appear in Figures 10,11,13,14,16 and 17. For $t = 0.1$ (short range) the particle and FEM solutions coincide for ϵ larger than 0.01 but a significant deviation appears for $\epsilon = 0.001$. This deviation between FEM and particle solution increases for larger t (longer ranges), and smaller ϵ. It is quite interesting to observe that for ϵ larger than 0.01 the FEM solution shows better agreement with the particle solution of the limit Wigner equation than with that of the Wigner equation itself. This indicates that in this range of frequencies, and for this particular potential, the solution is mainly driven by the initial field and not by the diffractive effects of the potential.

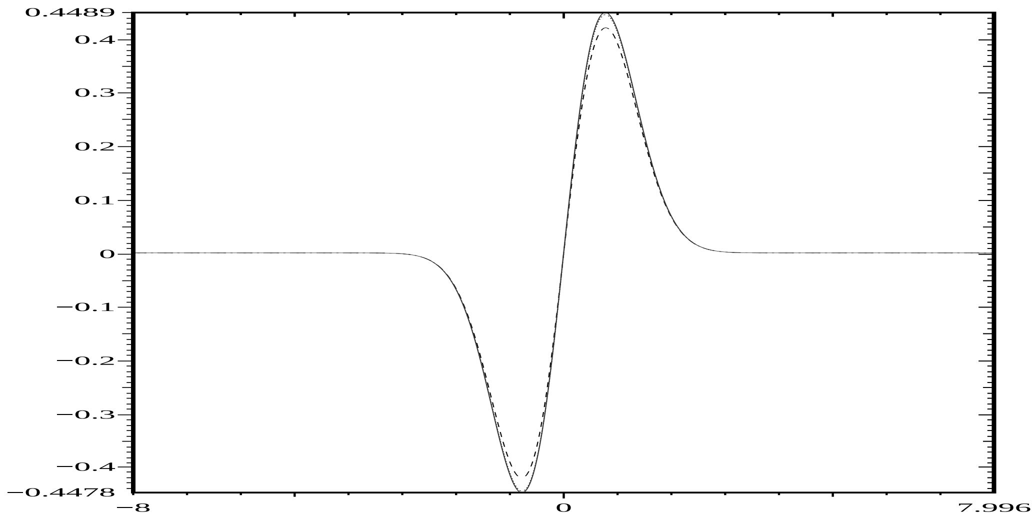


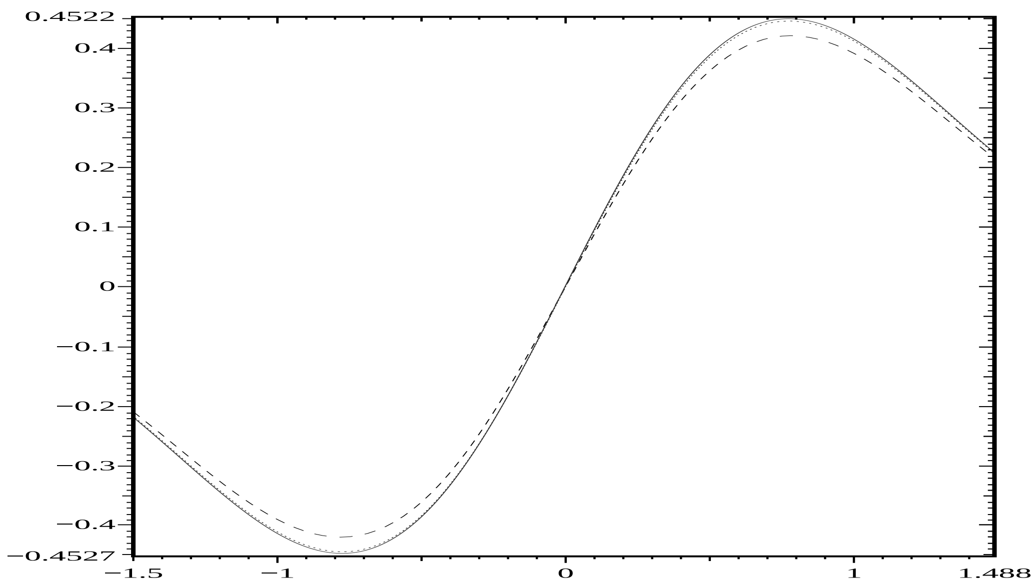


Figures $8a : |\psi_\epsilon(x, t = 0.1)|^2,\ \epsilon = 1\ vs.\ x$

$\#P = 90000\ Full\ Wigner(time = 750.95),\ Limit\ Wigner(time = 11.59),\ FEM(time = 67.08)$

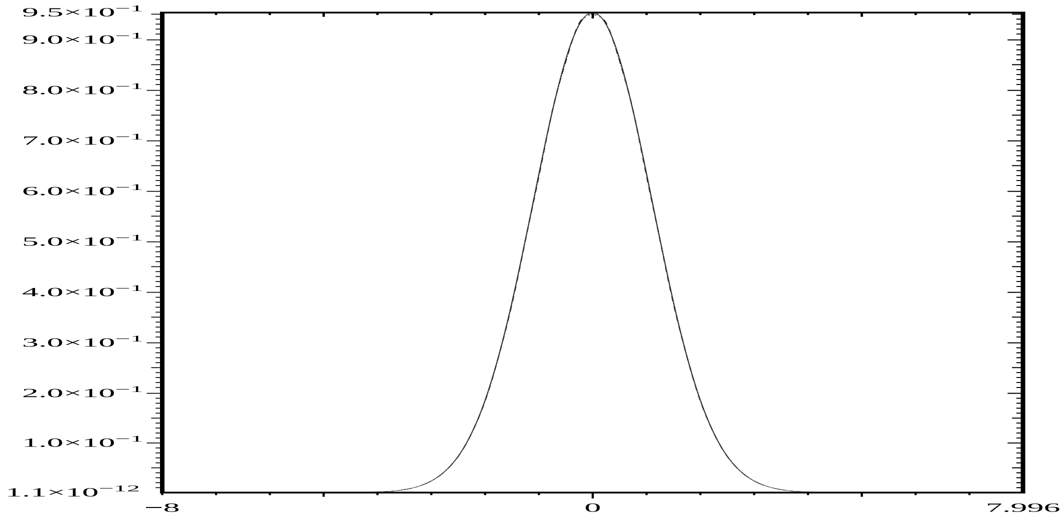
$(- - -\ Full\ Wigner\ Solution,\ \cdots\ Limit\ Wigner\ Solution,$—- $FEM\ Solution)$

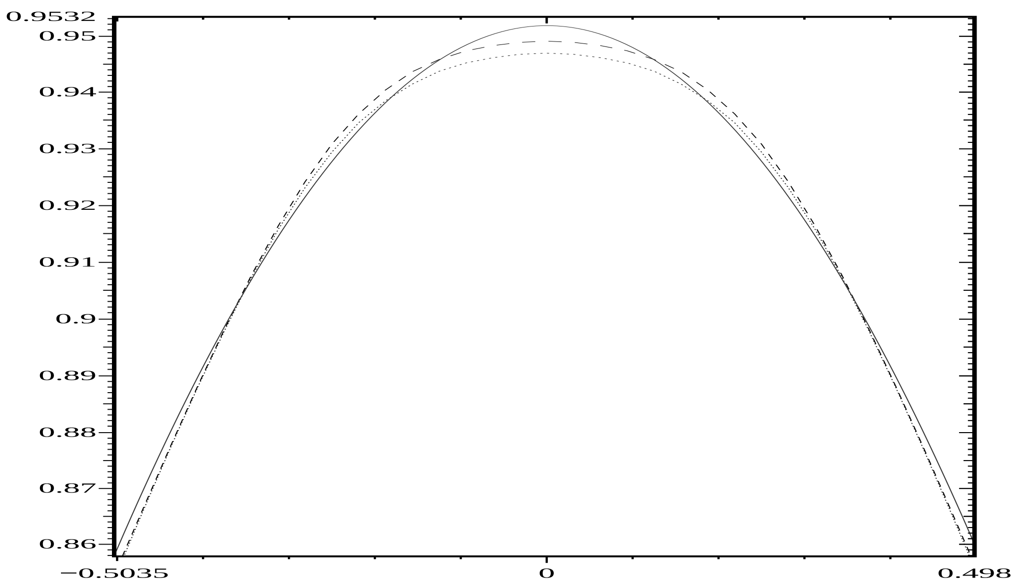




$$Figures\ 8b : \mathcal{F}(x,t=0.1),\ \epsilon = 1\ vs.\ x$$

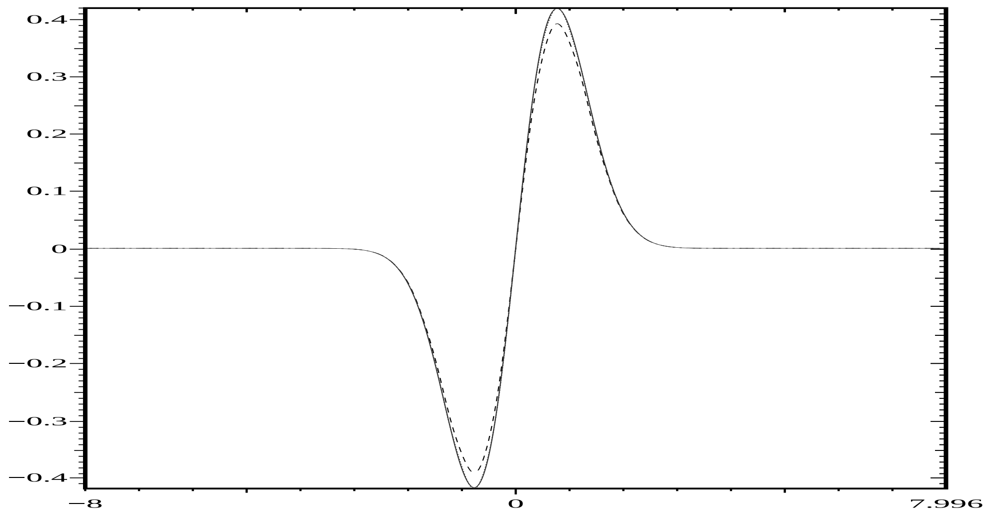
$\#P = 90000\ Full\ Wigner(time = 750.95),\ Limit\ Wigner(time = 11.59),\ FEM(time = 67.08)$

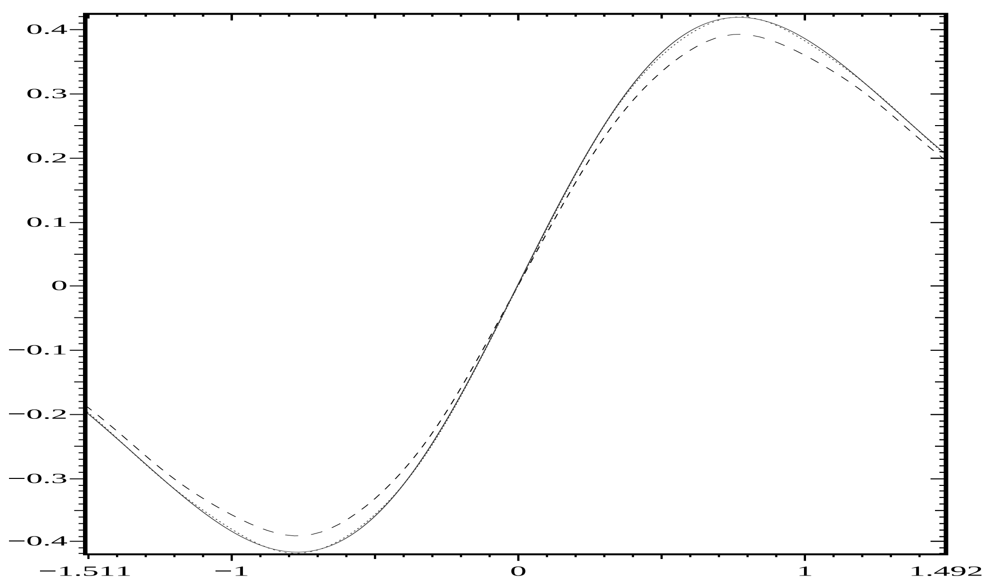




$$Figures\ 9a : |\psi_\epsilon(x, t = 0.1)|^2,\ \epsilon = 0.1\ vs.\ x$$

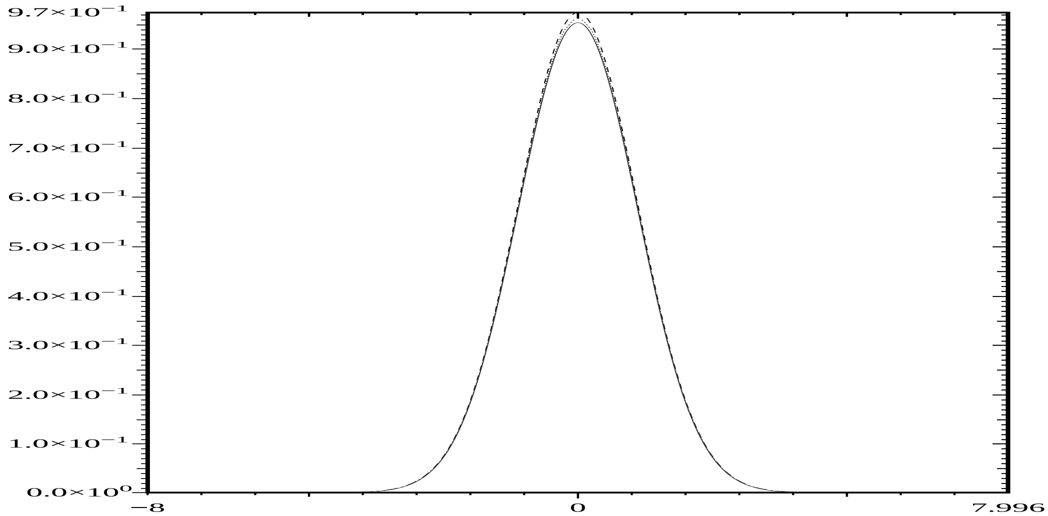
$\#P = 360000\ Full\ Wigner(time = 841.21)\ Limit\ Wigner(time = 49.28)\ FEM(time = 67.38)$

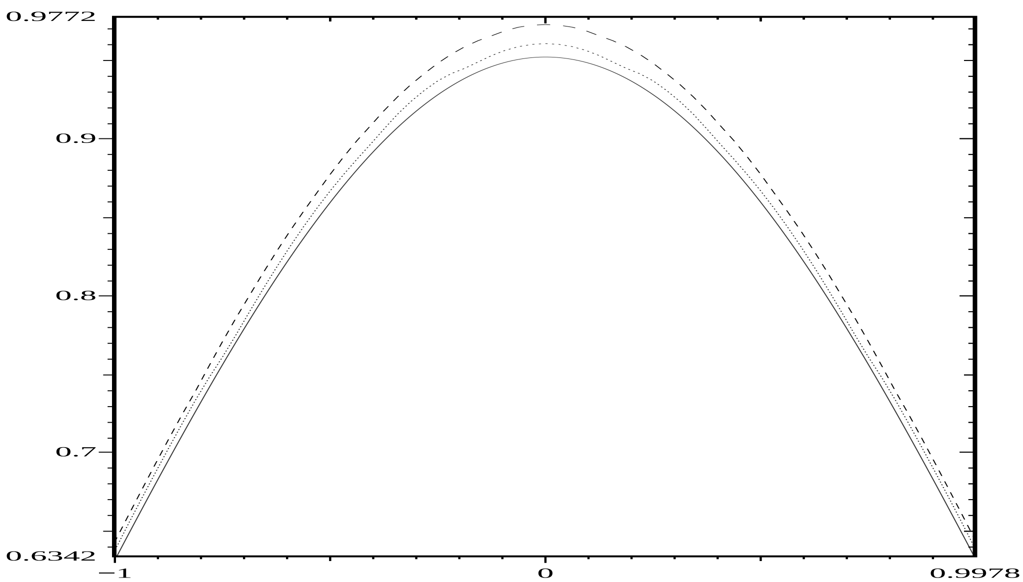




$Figures\ 9b : \mathcal{F}(x, t = 0.1),\ \epsilon = 0.1\ vs.\ x$

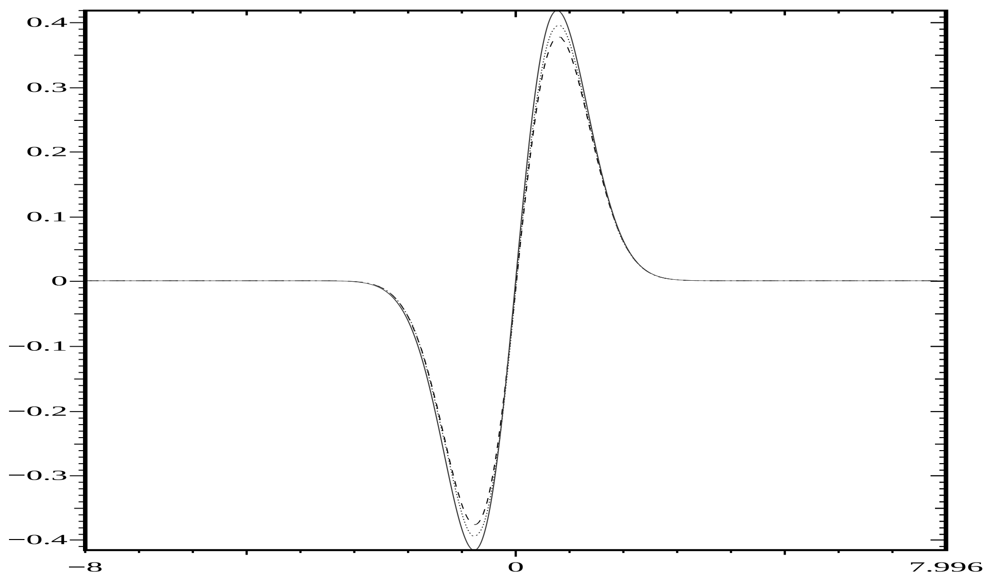
$\#P = 360000\ Full\ Wigner(time = 841.21)\ Limit\ Wigner(time = 49.28)\ FEM(time = 67.38)$





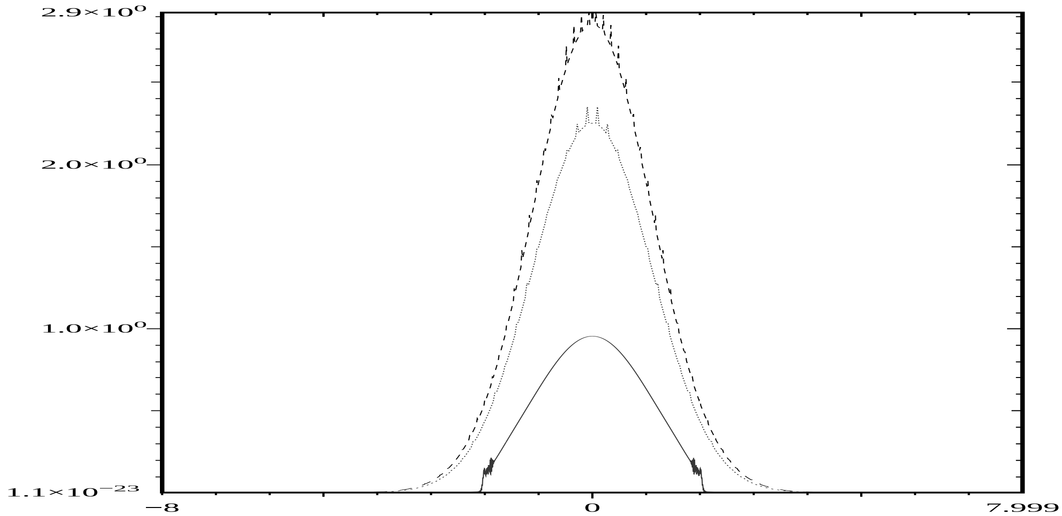
$$Figures\ 10a : |\psi_\epsilon(x, t = 0.1)|^2,\ \epsilon = 0.01\ vs.\ x$$

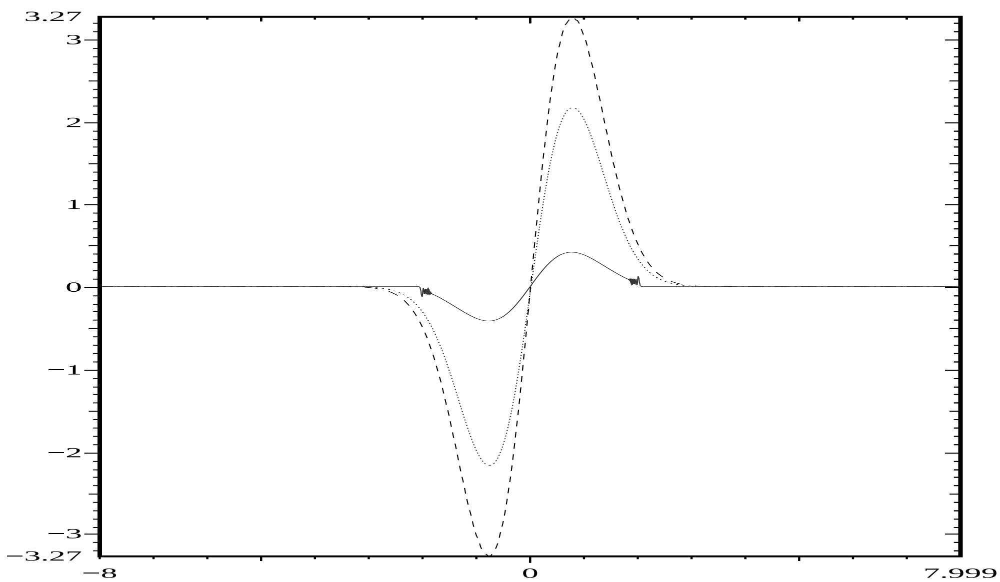
$Full\ Wigner(\#P = 1000000\ time = 2641.51),\ Limit\ Wigner(\#P = 1210000\ time = 164.97),\ FEM(time = 67.07)$



$$Figure\ 10b: \mathcal{F}(x, t = 0.1),\ \epsilon = 0.01\ vs.\ x$$

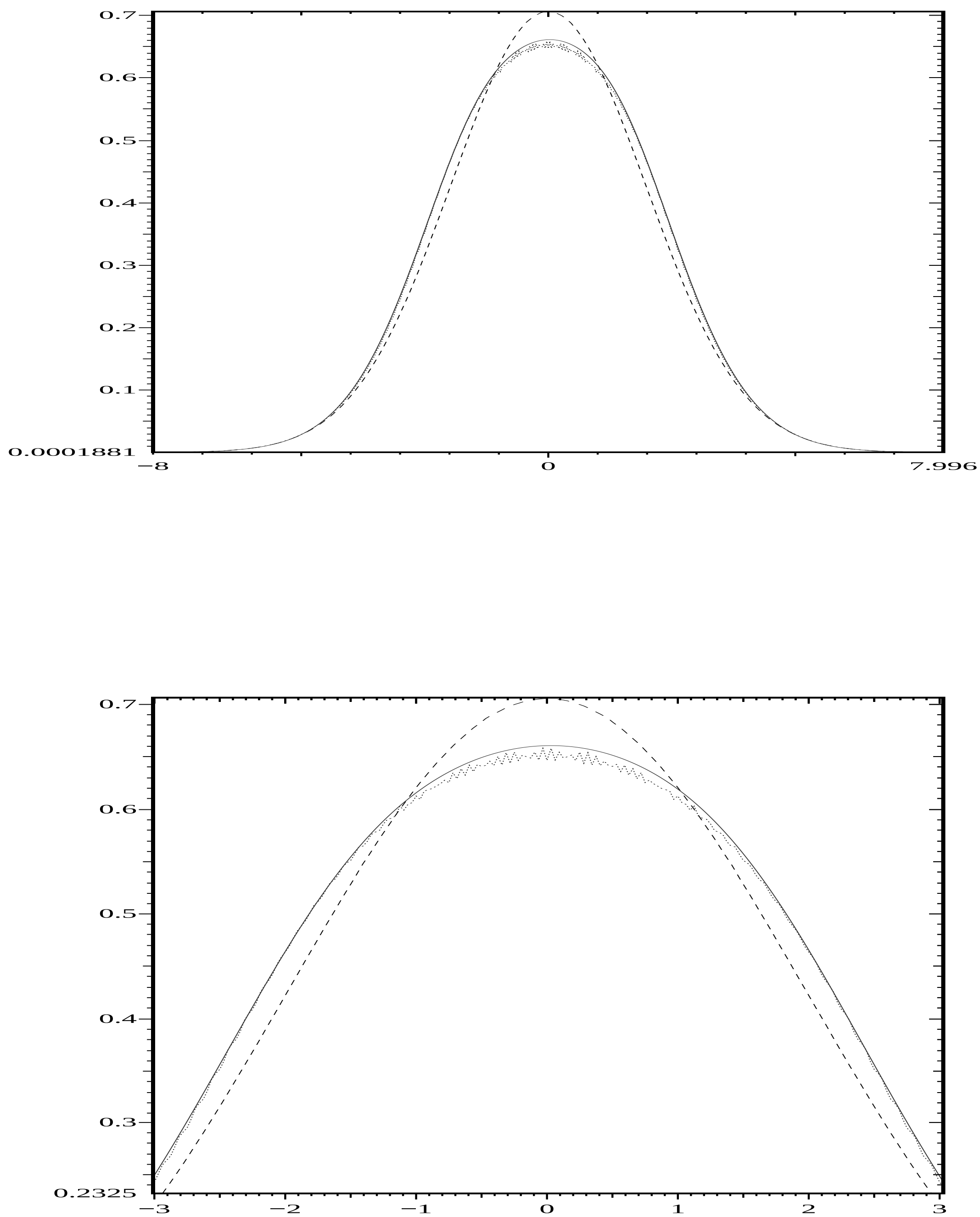
$Full\ Wigner(\#P = 1000000\ time = 2641.51), Limit\ Wigner(\#P = 1210000\ time = 164.97),\ FEM(time = 67.07)$





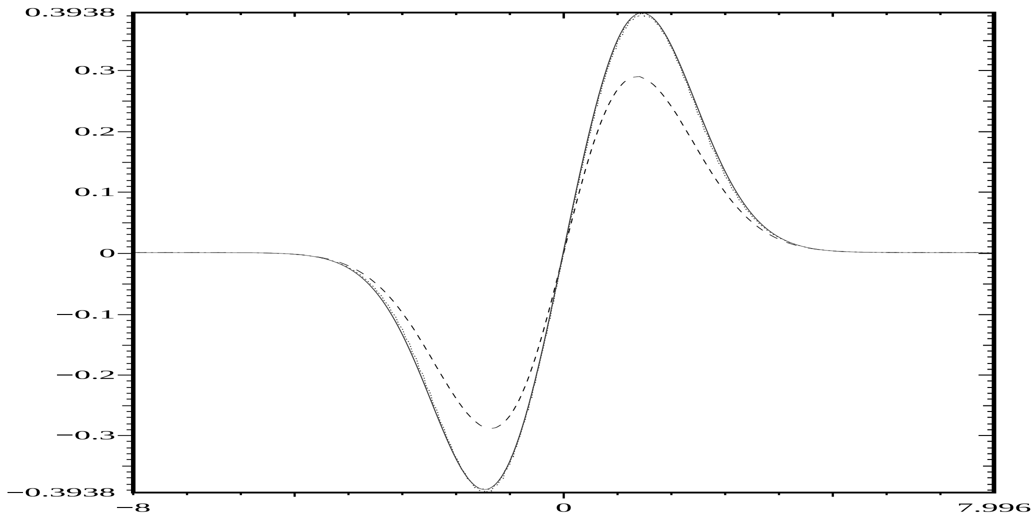
$Figures\ 11a : |\psi_\epsilon(x, t = 0.1)|^2,\ \mathcal{F}(x, t = 0.1),\ \epsilon = 0.001\ vs.\ x$

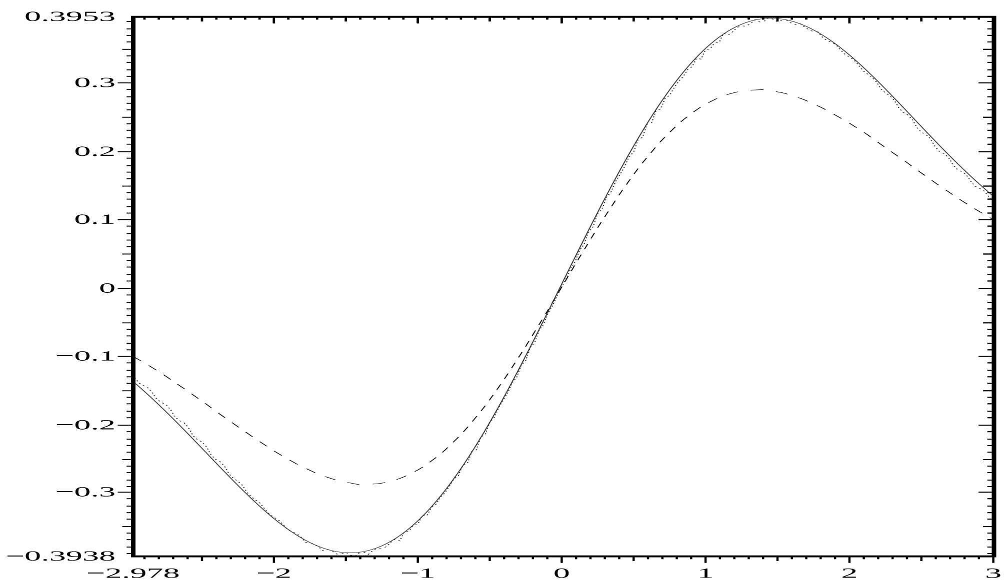
$Full\ Wigner(\#P = 1000000\ time = 11597.18),\ Limit\ Wigner(\#P = 2560000\ time = 349.79),\ FEM(time = 427.16)$



Figures $12a : |\psi_\epsilon(x, t = 0.8)|^2,\ \epsilon = 1\ vs.\ x$

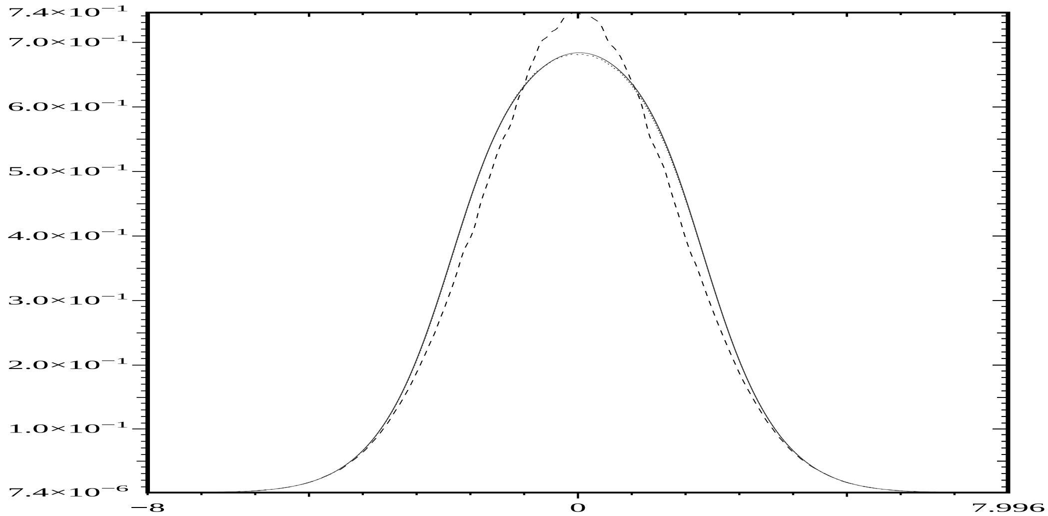
$\#P = 10000$ *Full Wigner*$(time = 84.08)$, *Limit Wigner*$(time = 8.27)$, *FEM*$(time = 67.17)$

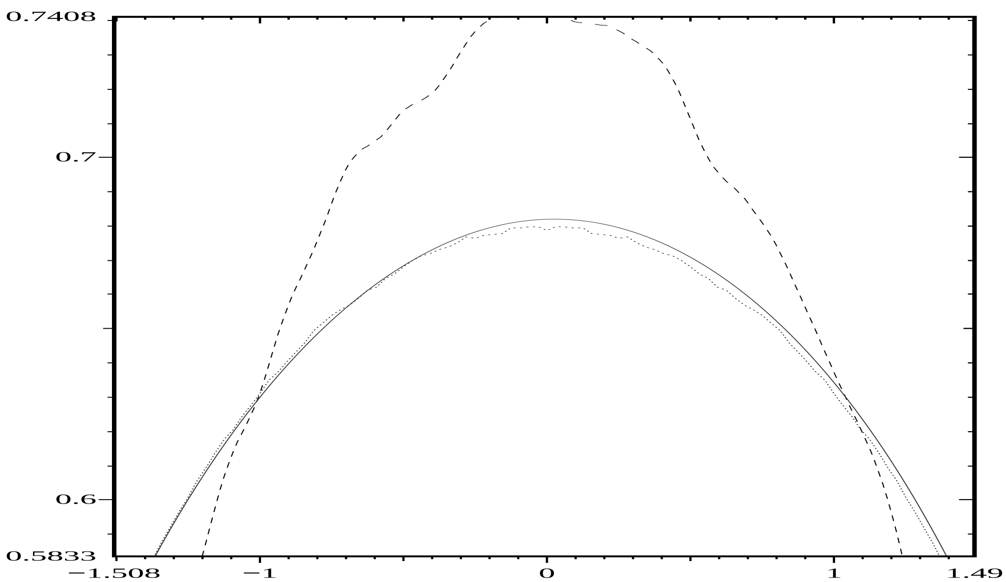




Figures $12b : \mathcal{F}(x, t = 0.8),\ \epsilon = 1\ vs.\ x$

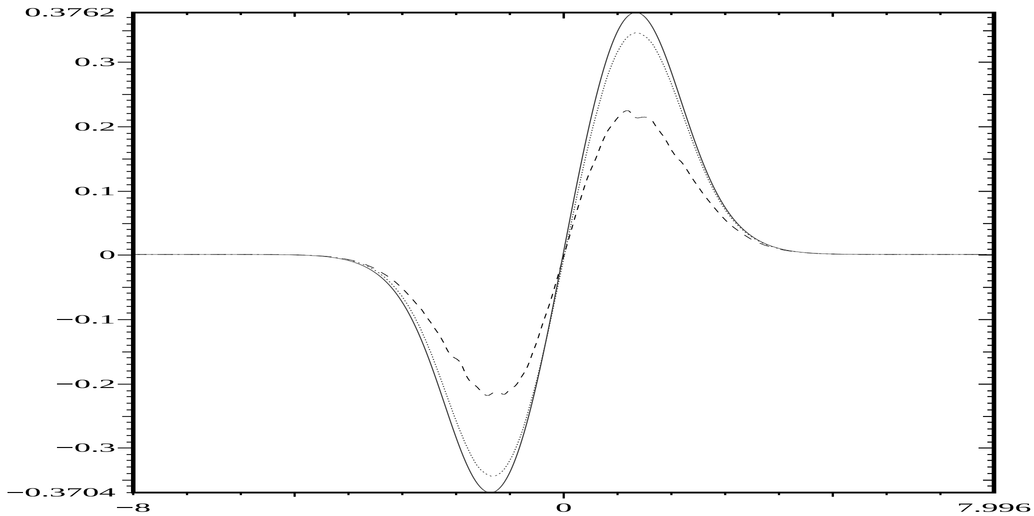
$\#P = 10000$ *Full Wigner*$(time = 84.08)$, *Limit Wigner*$(time = 8.27)$ *FEM*$(time = 67.17)$

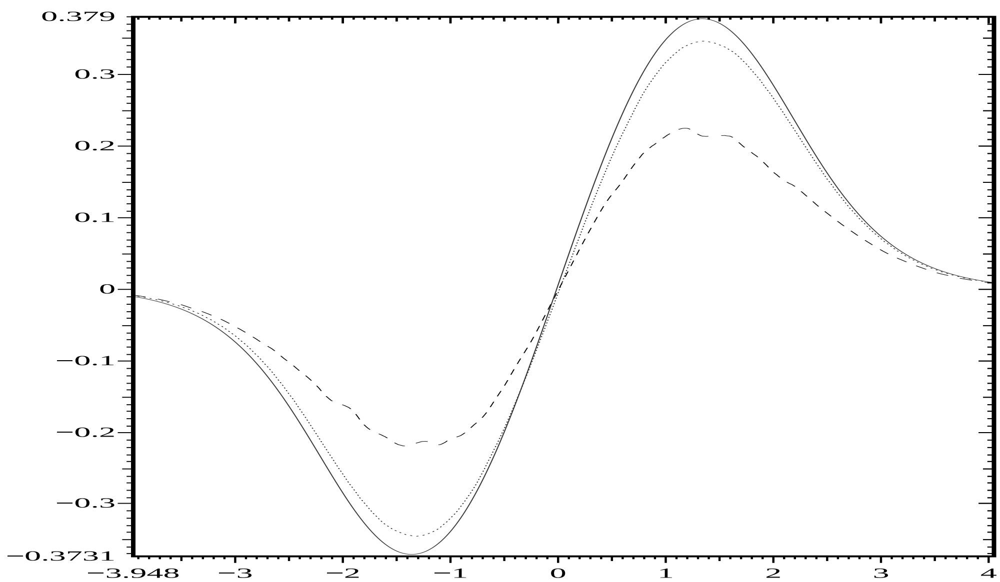




$Figures\ 13a : |\psi_\epsilon(x, t = 0.8)|^2, \epsilon = 0.1\ vs.\ x$

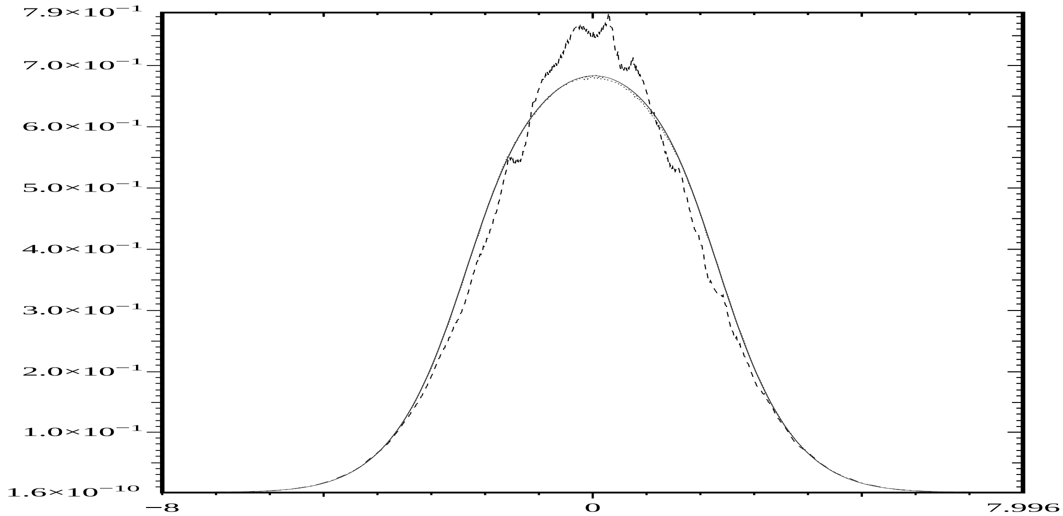
$\#P = 90000\ Full\ Wigner(time = 954.66),\ Limit\ Wigner(time = 74.0),\ FEM(time = 67.2)$

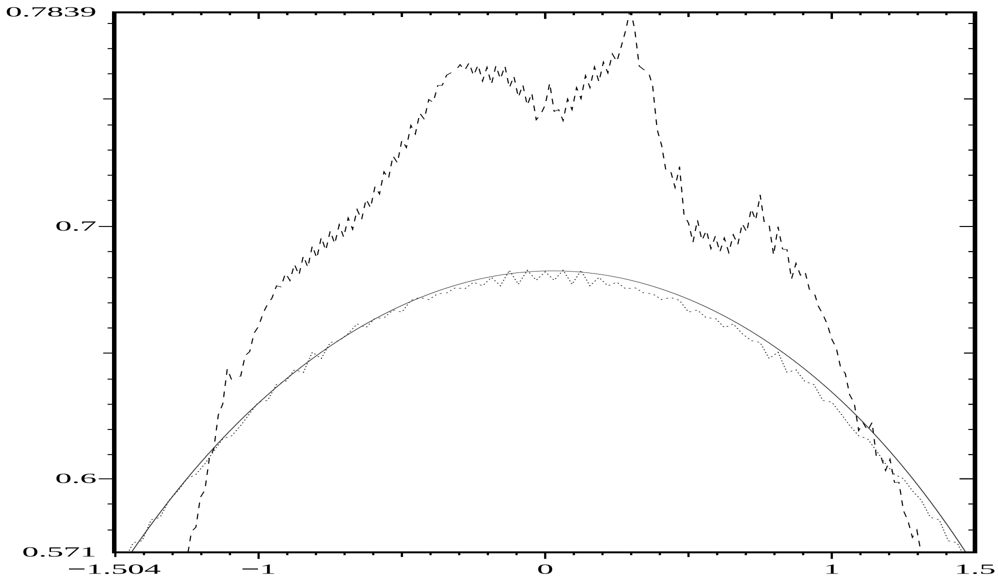




$Figures\ 13b : \mathcal{F}(x, t = 0.8),\ \epsilon = 0.1\ vs.\ x$

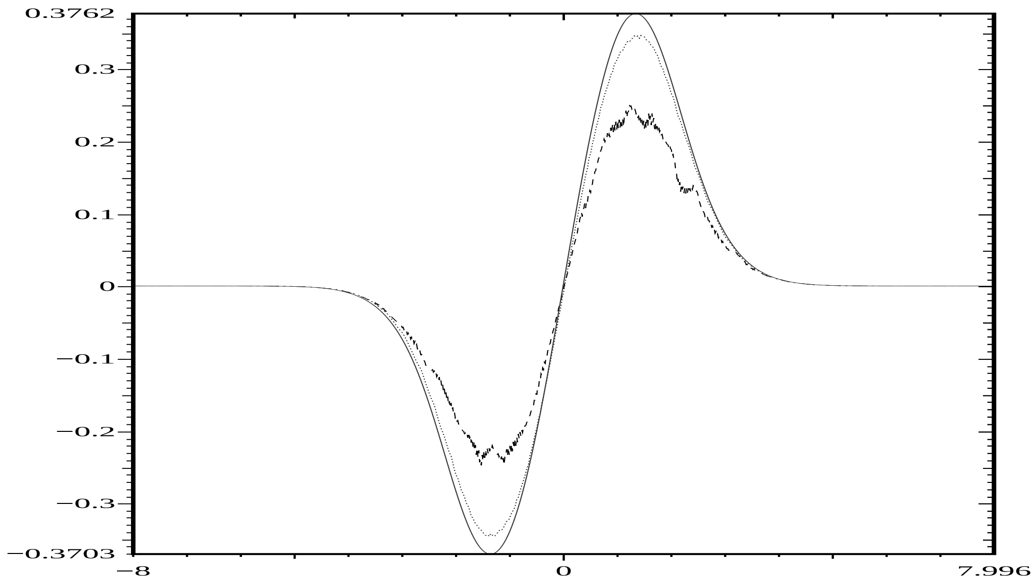
$\#P = 90000\ Full\ Wigner(time = 954.66),\ Limit\ Wigner(time = 74.0),\ FEM(time = 67.2)$





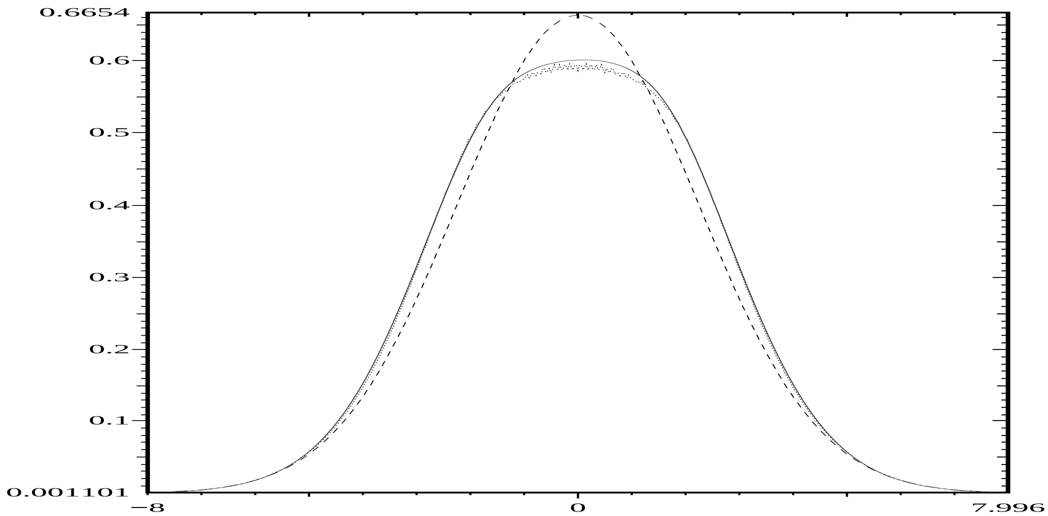
$Figures\ 14a : |\psi_\epsilon(x, t = 0.8)|^2,\ \epsilon = 0.01\ vs.\ x$

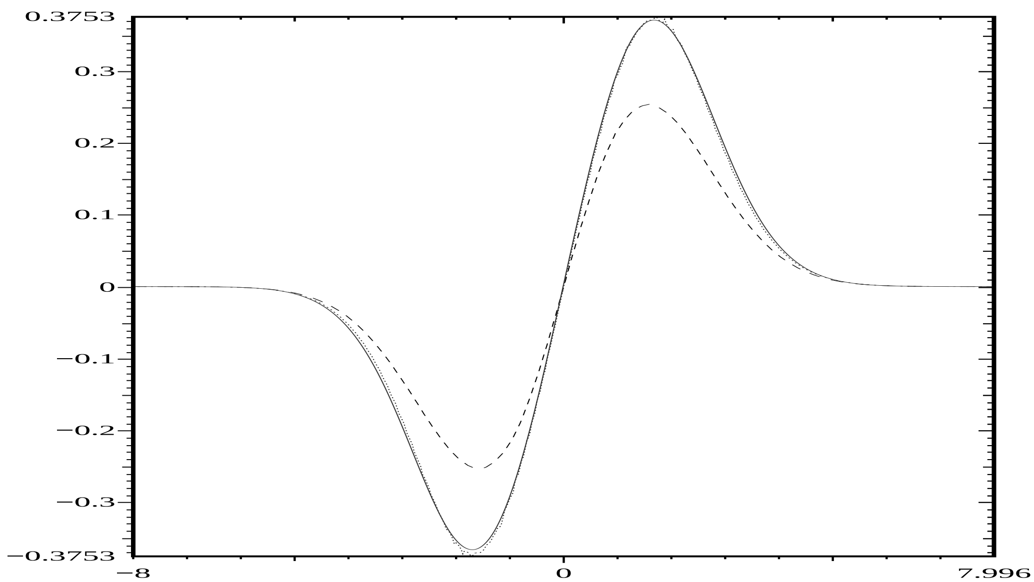
$Full\ Wigner(\#P = 810000\ time = 8503.96),\ Limit\ Wigner(\#P = 2560000\ time = 2125.21),\ FEM(time = 67.30)$



$Figure\ 14b : \mathcal{F}(x,t=0.8),\ \epsilon=0.01\ vs.\ x$

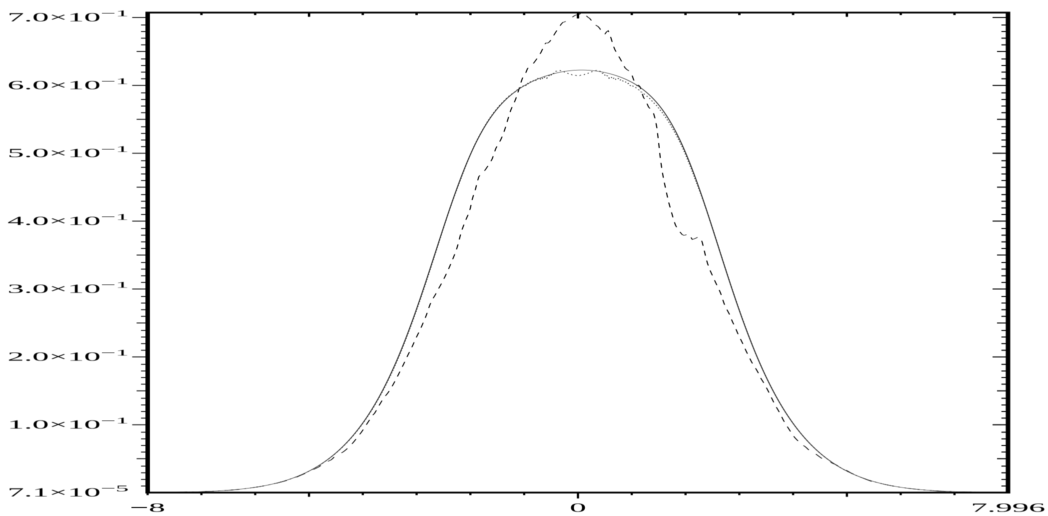
$Full\ Wigner(\#P = 810000\ time = 8503.96),\ Limit\ Wigner(\#P = 2560000\ time = 2125.21),\ FEM(time = 67.30)$

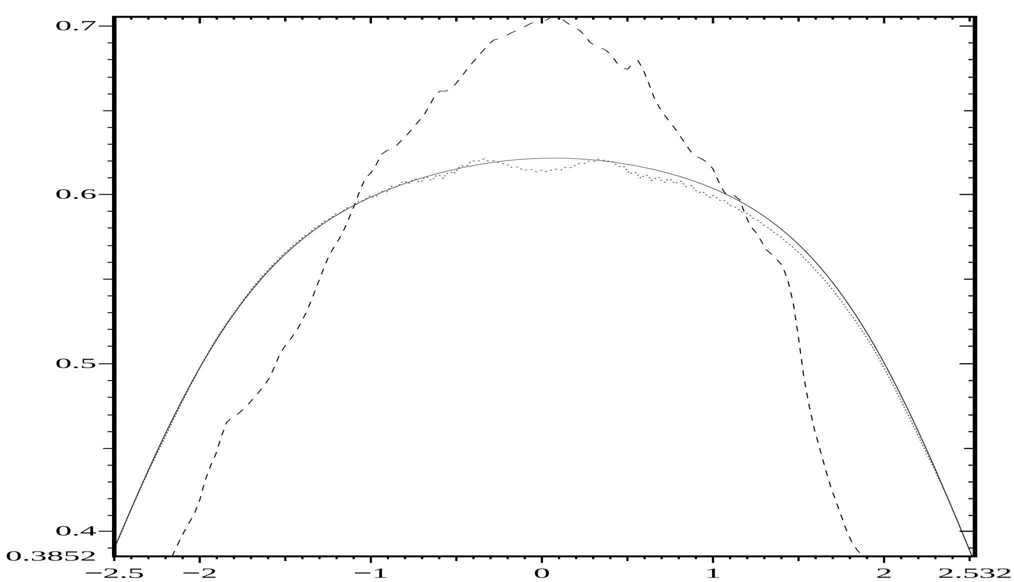




$Figures\ 15a : |\psi_\epsilon(x, t = 1)|^2,\ \mathcal{F}(x, t = 1),\ \epsilon = 1\ vs.\ x$

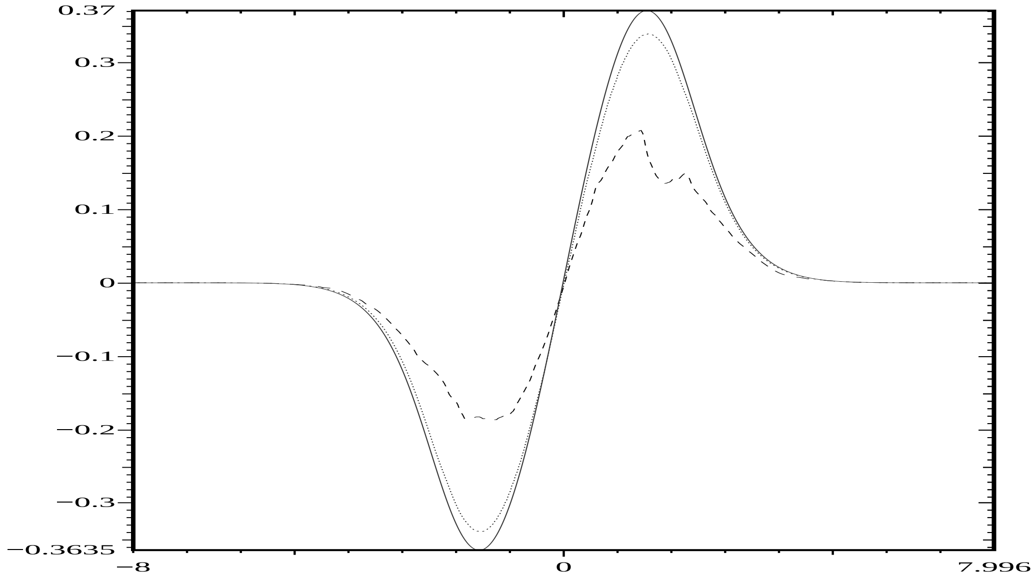
$\#P = 10000\ Full\ Wigner(time = 22.05),\ Limit\ Wigner(time = 10.12),\ FEM(time = 66.84)$





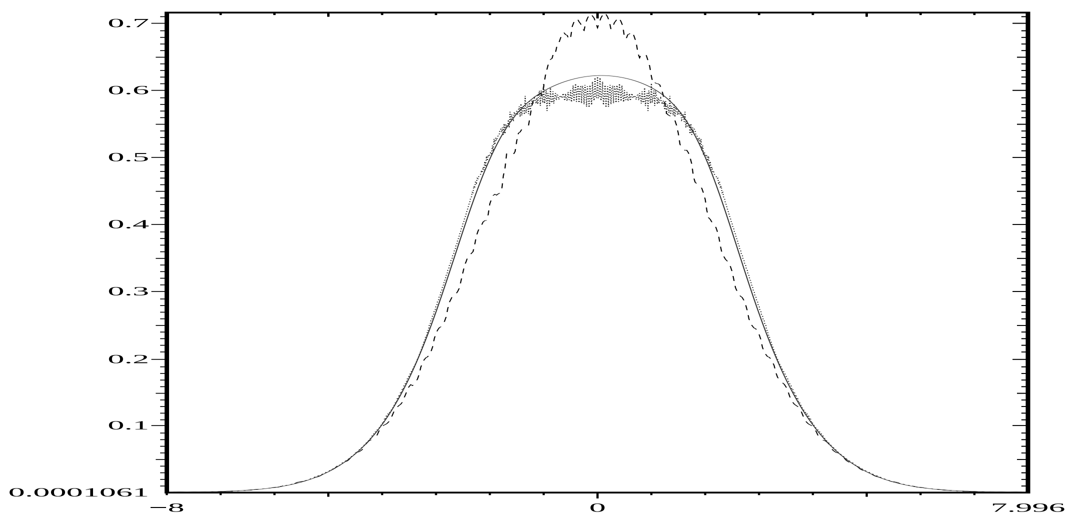
$$Figures\ 16a : |\psi_\epsilon(x,t=1)|^2,\ \epsilon = 0.1\ vs.\ x$$

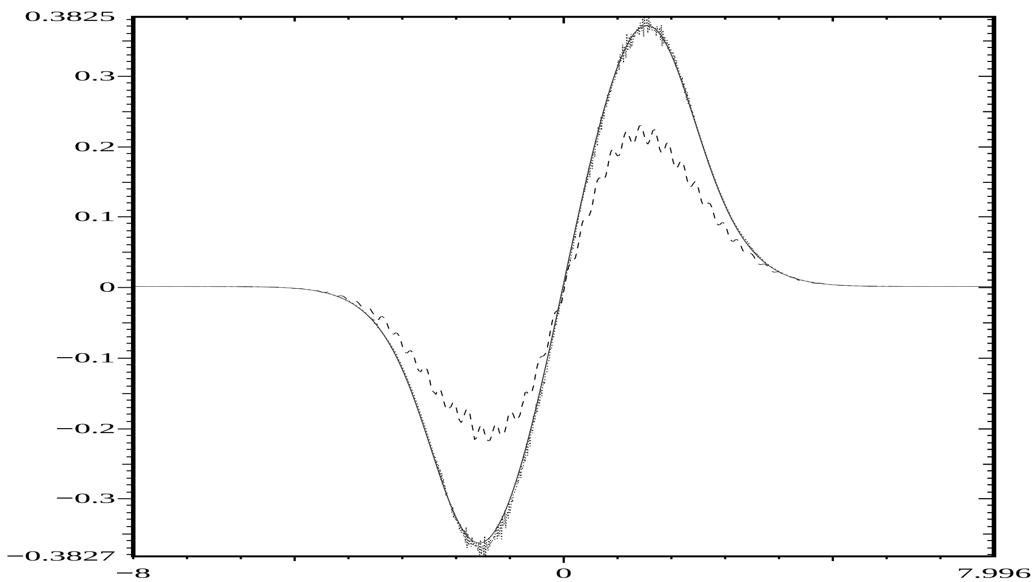
$\#P = 90000\ Full\ Wigner(time = 198.32),\ Limit\ Wigner(time = 163.39),\ FEM(time = 66.84)$



$Figure\ 16b : \mathcal{F}(x, t = 1),\ \epsilon = 0.1\ vs.\ x$

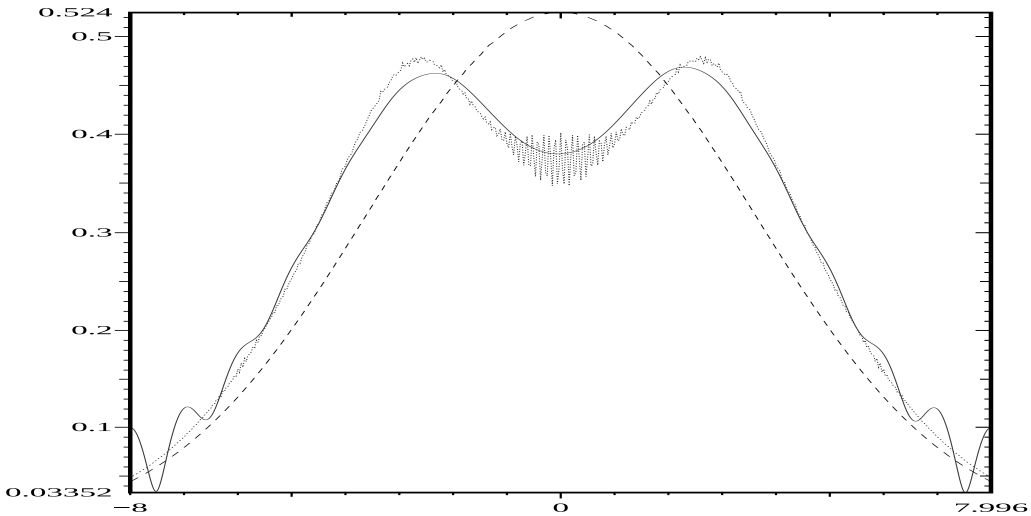
$\#P = 90000\ Full\ Wigner(time = 198.32),\ Limit\ Wigner(time = 163.39),\ FEM(time = 66.84)$

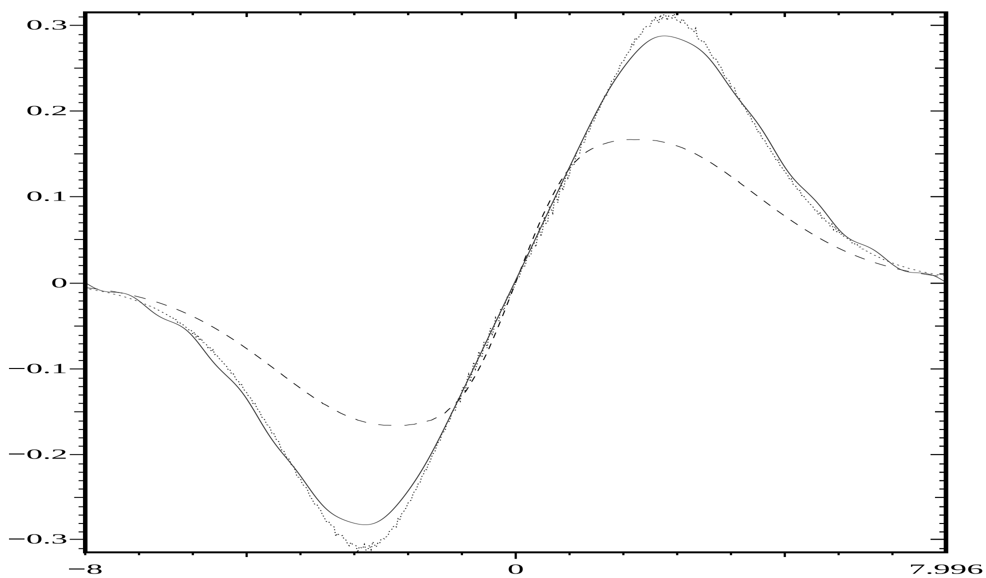




$$Figures\ 17a : |\psi_\epsilon(x,t=1)|^2, \quad \mathcal{F}(x,t=1)\ \epsilon = 0.01\ vs.\ x$$

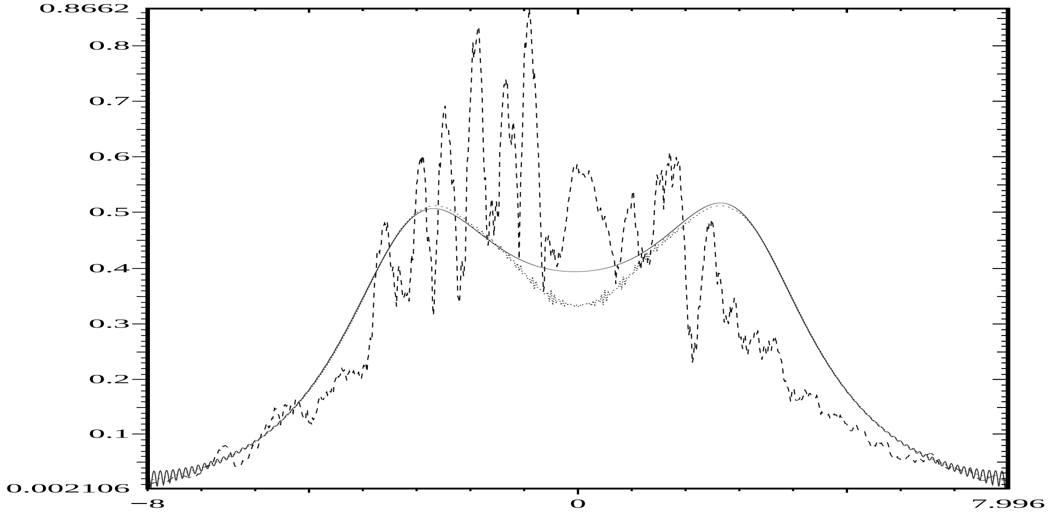
$\#P = 810000$ $Full\ Wigner(time = 1959.65),\ Limit\ Wigner(time = 1661.21),\ FEM(time = 66.8)$

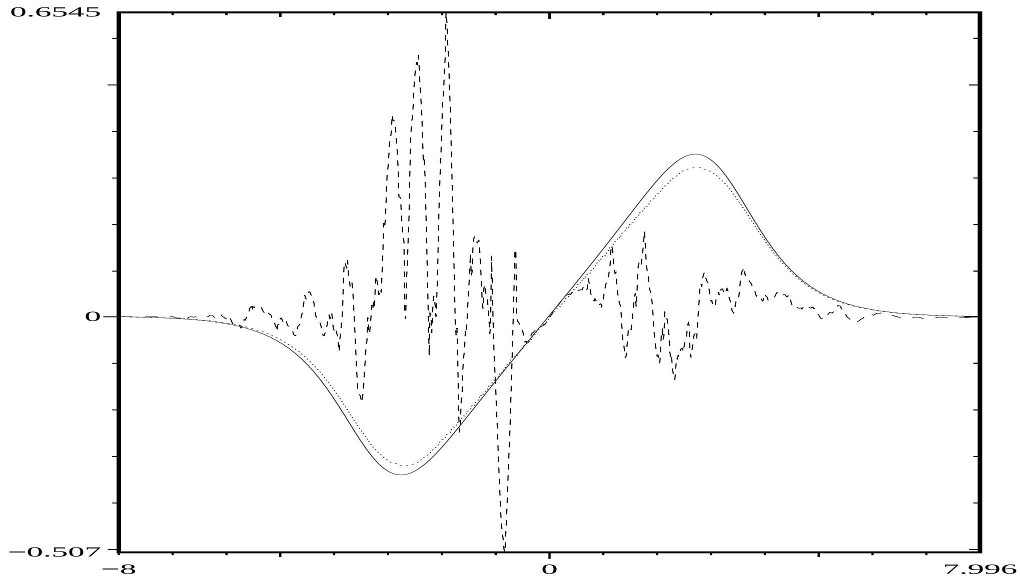




$Figures\ 18a : |\psi_\epsilon(x,t=2)|^2, \quad \mathcal{F}(x,t=2)\ \epsilon=1\ vs.\ x$

$Full\ Wigner(\#P\ =\ 40000\ time\ =\ 490.68),\ Limit\ Wigner(\#P\ =\ 250000\ time = 506.06),\ FEM(time = 66.83)$





$$Figures\ 19a: |\psi_\epsilon(x,t=2)|^2, \quad \mathcal{F}(x,t=2)\ \epsilon = 0.1\ vs.\ x$$

$\#P = 810000\ Full\ Wigner(time = 9928.25),\ Limit\ Wigner(time = 1637.01),\ FEM(time = 66.87)$

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