Using an *r*-dependent Gaussian width in calculations of the globally uniform semiclassical wave function

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The globally uniform semiclassical wave function expresses the solution to the time independent Schrödinger equation in terms of fixed width Gaussian wave packets traveling along a set of trajectories. There is a globally uniform wave function (GUWF) for each value of the Gaussian width parameter γ. Numerical data show that a small Gaussian width is needed in some regions to obtain accurate results, while a broad Gaussian width provides better results in other regions. Since there is a semiclassically valid GUWF for every positive value of γ, it is reasonable to employ the GUWF corresponding to a Gaussian width that provides good results at each value of $\mathbf{r}$. A criterion for the $\mathbf{r}$ dependent choice of γ is proposed and tested on one and two dimensional model problems. The results show that the use of an $\mathbf{r}$ dependent γ in the GUWF results in improved accuracy for the model problems considered. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2424938]

I. INTRODUCTION

Semiclassical methods[1–20] represent a useful middle ground between quantum mechanical calculations, which rapidly become numerically too demanding as the dimensionality of the problem increases, and classical mechanical calculations, which neglect often important quantum interference effects. Primitive semiclassical approximations[3–5,21] suffer from the fact that they have singularities at turning points and caustics in the classical motion. They also require that trajectories be found that obey specific initial and final conditions, which is a numerically difficult task. The globally uniform wave function[7–9] (GUWF) is a time independent semiclassical wave function that does not suffer from these numerical drawbacks. The GUWF, which expresses the wave function in terms of frozen Gaussian wave packets traveling along classical trajectories, is given by

$$\psi_E(\mathbf{r}, \gamma) = N \int d\mathbf{s} \, C(\mathbf{s}) g_\gamma(\mathbf{r}; \mathbf{r}_t, \mathbf{p}_t) e^{iw(\mathbf{r}_t)}, \tag{1}$$

where E is the energy, N defines the overall normalization of the wave function, $g_\gamma(\mathbf{r}; \mathbf{r}_t, \mathbf{p}_t)$ has the form

$$\begin{aligned} g_\gamma(\mathbf{r}; \mathbf{r}_t, \mathbf{p}_t) = (2\gamma_R/\pi\hbar)^{n/4} \\ \times \exp[-(\gamma/\hbar)(\mathbf{r} - \mathbf{r}_t)^2 + i(\mathbf{p}_t/\hbar) \cdot (\mathbf{r} - \mathbf{r}_t)], \end{aligned} \tag{2}$$

in n dimensions, $\gamma_R = \mathrm{Re}(\gamma)$, and

$$w(\mathbf{r}_t) = \int_{\mathbf{r}_0}^{\mathbf{r}_t} \mathbf{p} \cdot d\mathbf{r}. \tag{3}$$

In this work, γ is taken to be real. The integration in Eq. (1) is over an appropriate set of trajectories and over the time along the trajectory. For example, in a simple two body central field scattering problem in n dimensions where the only coordinates are the relative positions of the two particles (i.e., the particles have no internal degrees of freedom) and

where the incoming wave function is a plane wave, each trajectory can be specified by a point on a plane in the incoming asymptotic region which is perpendicular to the incoming asymptotic momentum $\mathbf{p}_0$. This point, $\mathbf{r}_0$ and the momentum $\mathbf{p}_0$ define the phase space point for the trajectory at $t=0$. The $\mathbf{s}$ integration in Eq. (1) is over the time (i.e., $s_1=t$ with $-\infty < s_1 < \infty$) and over $n-1$ other coordinates, s_2, $s_3, \ldots, s_n$, that determine the location of $\mathbf{r}_0$ in the asymptotic plane. The prefactor $C(\mathbf{s})$ is given by $[\det(\mathbf{B})]^{1/2}$, where $\mathbf{B} = \partial \mathbf{p}_t/\partial \mathbf{s} - 2i\gamma \partial \mathbf{r}_t/\partial \mathbf{s}$, and the integration in Eq. (3) is performed along the trajectory that starts at $\mathbf{r}_0$.

There is a globally uniform wave function for each positive value of the width parameter γ. A relatively small γ might be a good choice in some regions of $\mathbf{r}$, while a larger γ may be needed in other regions. Since $\psi_E(\mathbf{r}, \gamma)$ is a uniform semiclassical wave function for any choice of γ, there is no reason why one could not use different $\psi_E(\mathbf{r}, \gamma)$ in different regions. The usefulness of this suggestion is explored in this paper. In choosing a γ, several criteria are considered. First, the method of selecting the γ for each $\mathbf{r}$ should not significantly increase the computational effort of the method. For instance, the fixed γ calculation of $\psi_E(\mathbf{r}, \gamma)$ requires that the equations of motion for $\mathbf{r}$, $\mathbf{p}$, $\mathbf{M}_{rr}$, and $\mathbf{M}_{pr}$ be integrated along classical trajectories, where $\mathbf{M}_{rr} = \partial \mathbf{r}_t/\partial \mathbf{r}_0$ and $\mathbf{M}_{pr} = \partial \mathbf{p}_t/\partial \mathbf{r}_0$. The selection procedure for γ at each $\mathbf{r}$ should not, for example, contain derivatives of the stability matrices $\mathbf{M}_{rr}$ and $\mathbf{M}_{pr}$ with respect to $\mathbf{r}_0$, as this would significantly increase the number of quantities that would have to be integrated along the trajectories. In addition, one expects that large values of γ increase the numerical effort, since this corresponds to very narrow Gaussians, and this would necessitate the use of a very narrowly spaced set of trajectories in order to accurately numerically perform the integrations in Eq. (1). If these integrations are performed using a Monte Carlo procedure, this would result in the need for a very large sample. The numerical examples shown below demonstrate that a relatively large γ may be required to
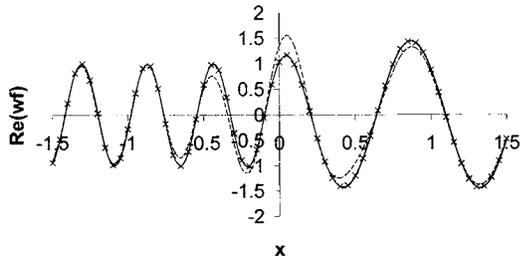
FIG. 1. The real part of $\psi(x)$ for $E=1.3$ and $V(x)$ given by Eq. (4) with $m=80$ and $\hbar=1$, (——) quantum wave function, (----) GUWF with $\gamma=1$, and ($\times\times\times$) primitive wave function.

achieve accurate results using the GUWF for some $\mathbf{r}$, while a smaller γ is sufficient in other regions. If a selection procedure of γ can be devised that chooses a different γ for different regions, then the numerical routine for the integrations in Eq. (1) could be adapted to use a finer grid of trajectories only in those regions where this is needed.

Consider the one dimensional model problem with

$$V(x) = [\tanh(5x) + 1]/2, \qquad (4)$$

with a particle mass of 80, $\hbar=1$, and $E=1.3$. The quantum, primitive semiclassical, and globally uniform wave functions with a width parameter $\gamma=1$ are plotted in Fig. 1. The primitive wave function is given by[3,21]

$$\psi_E^{pr}(\mathbf{r}) = [|\det(\partial\mathbf{r}_t/\partial\mathbf{r}_0)|]^{-1/2}e^{i(w+w_0)/\hbar-n_ci\pi/2}, \qquad (5)$$

where this expression is evaluated for trajectories that begin at $\mathbf{r}_0$ in the incoming asymptotic region with the appropriate initial momentum and end at $\mathbf{r}$. The phase function w is given by Eq. (3) with the upper limit of $\mathbf{r}$, w_0 is a constant, and n_c is the Maslov index.[23] Details of these calculations are provided in Sec. III. The interesting feature of the data in Fig. 1 is that the primitive semiclassical wave function reproduces the quantum result very well while the GUWF is less accurate near $x=0$ for this value of γ. In the large γ limit the Gaussian wave packets approach $(2\pi\hbar/\gamma)^{n/4}\delta(\mathbf{r}-\mathbf{r}_t)$, where $\delta(\mathbf{r})$ is the Dirac delta function, and the GUWF approaches the primitive semiclassical wave function. Given that the primitive wave function is more accurate than the GUWF for some x, one would expect that the globally uniform result can be improved by increasing γ for values of x at which the GUWF is less accurate.

In the next section a criterion for choosing an appropriate value of γ at each $\mathbf{r}$ is presented. This procedure is tested for this one dimensional model and for a two dimensional model problem in Sec. III. The results are discussed and summarized in Sec. IV.

II. CRITERION FOR CHOOSING THE GAUSSIAN WIDTH

Semiclassical wave functions are generally expressed as a prefactor multiplied by an exponential of the form $e^{f/\hbar}$ or as integrals with an integrand of this form. Since a semiclassical approximation is a small $\hbar$ approximation, the factor of $1/\hbar$ in the exponential implies that the $e^{f/\hbar}$ is changing much more rapidly than the prefactor. Due to the form of f for the GUWF, $f(\mathbf{s})=-\gamma(\mathbf{r}-\mathbf{r}_t)^2+i\mathbf{p}_t(\mathbf{r}-\mathbf{r}_t)+iw(\mathbf{r}_t)$, only values of $\mathbf{s}$

for which $\mathbf{r}_t$ is close to $\mathbf{r}$ contribute significantly to $\psi_E(\mathbf{r},\gamma)$. The condition that the prefactor $C(\mathbf{s})$ should be a relatively slowly varying quantity suggests that γ be chosen so that $C(\mathbf{s})$ does not change too much over the width of the Gaussian functions given by Eq. (2). The logarithmic derivative of $C(\mathbf{s})$ with respect to s_j is given by

$$\frac{1}{C}\frac{\partial C}{\partial s_j} = \frac{1}{2}\mathrm{Tr}\,\mathbf{B}^{-1}\frac{\partial\mathbf{B}}{\partial s_j}, \qquad (6)$$

where Tr indicates the trace operation. In a one dimensional problem, this derivative becomes $(1/2)(\partial^2 q/\partial s^2)/(\partial q/\partial s)$, where $q=p_t-2i\gamma r_t$. If the integration variable s is changed from the time along the trajectory to the distance along the trajectory, then this quantity has dimensions of inverse length. The condition that the prefactor is slowly changing on the length scale of the Gaussian width suggests that γ should be chosen such that the dimensionless quantity $(\hbar/4\gamma)|(\partial^2 q/\partial s^2)/(\partial q/\partial s)|^2$ is small. Thus,

$$\gamma = c_1|\partial^2 q_t/\partial x_t^2|^2/[|\partial q_t/\partial x_t|^2 + c_2] \qquad (7)$$

is used to select the value of γ as a function of x for one dimensional problems in this work. Equation (7) results in a cubic equation for γ. If there are three real roots of this equation, the largest of them is used. The constant c_1 is taken to be $2\hbar$ and the constant c_2 is set to 0.1 throughout this work. The constant c_2 is added in anticipation of the possibility of the analog of $|\partial q_t/\partial x_t|^2$ having zeros in multidimensional problems, resulting in unnecessarily large values of γ. In addition, the choice of γ is restricted to be between a minimum value $\gamma_{\min}$ and a maximum value $\gamma_{\max}$. The constant c_2 has the same dimensions as γ^2. It can be made dimensionless by replacing c_2 in Eq. (7) with $c_2\gamma_{\min}^2$. γ is also required to be of the form $\gamma_k=2^k\gamma_{\min}$, where k is an integer. If Eq. (7) yields a γ between $\gamma_{\min}$ and $\gamma_{\max}$, then the smallest γ_k that is larger than the γ given by Eq. (7) is employed. Values of $\gamma_{\min}=1$ and $\gamma_{\max}=2^9\gamma_{\min}$ are employed in all calculations in this work. The restriction of γ to a discreet set of values is imposed for numerical reasons. The sign of the square root in the prefactor $C=[\det(\mathbf{B})]^{1/2}$ is chosen so that the prefactor changes continuously along the trajectory. As the trajectory is run in the calculation, the prefactors for the ten values of gamma corresponding to $n=0,1,\ldots,9$ are evaluated at each step to assure their continuity as a function of time. The appropriate prefactor can then be used at each point x at which the wave function is evaluated. An alternative possibility would be to select γ using Eq. (7), rather than limiting it to one of the γ_k when γ is between $\gamma_{\min}$ and $\gamma_{\max}$, and then use the known values of the prefactors at the nearest values of γ_k in determining the sign of the prefactor at the selected γ. This would result in a γ that varied smoothly with $\mathbf{r}$.

Suppose that $C(\mathbf{s})$ is slowly changing at $\mathbf{r}$, resulting in a relatively small γ from Eq. (7). This value of γ would result in a range of $\mathbf{s}$ corresponding to a fairly large spread in $\mathbf{r}_t$ contributing significantly to the integrand in Eq. (1). It is possible that $C(\mathbf{s})$ is changing more rapidly at other points in this range, producing a relatively large overall change in $C(\mathbf{s})$ over the range of $\mathbf{s}$ that contribute significantly to $\psi_E(\mathbf{r},\gamma)$. The use of a larger value of γ is probably appro-
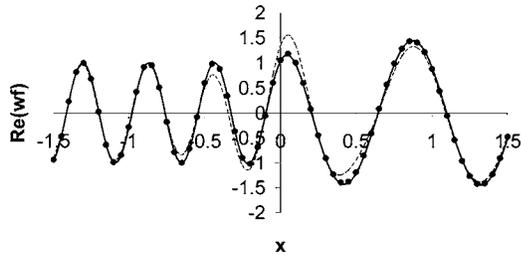
FIG. 2. The real part of $\psi(x)$ for $E=1.3$ and $V(x)$ given by Eq. (4) with $m=80$ and $\hbar=1$; (——) quantum wave function, (----) GUWF with $\gamma=1$, and ($\cdots$) variable γ GUWF.

TABLE I. The values of γ for the variable γ globally uniform wave function at various x for the one dimensional problem.

x	γ	x	γ	x	γ
−2.5	1	−0.8	8	0.9	8
−2.4	1	−0.7	16	1.0	8
−2.3	1	−0.6	16	1.1	8
−2.2	1	−0.5	32	1.2	8
−2.1	1	−0.4	32	1.3	4
−2.0	2	−0.3	32	1.4	4
−1.8	2	−0.2	32	1.5	4
−1.8	2	−0.1	32	1.6	2
−1.7	2	0.0	32	1.7	2
−1.6	2	0.1	32	1.8	2
−1.5	4	0.2	32	1.9	2
−1.4	4	0.3	32	2.0	2
−1.3	4	0.4	32	2.1	2
−1.2	4	0.5	32	2.2	1
−1.1	8	0.6	32	2.3	1
−1.0	8	0.7	16	2.4	1
−0.9	8	0.8	16	2.5	1

priate in this case. For this reason, estimates of γ from points near $\mathbf{r}$ are obtained when selecting the value of γ at $\mathbf{r}$. A point $\mathbf{r}_1$ is considered to be near $\mathbf{r}$ if $(\mathbf{r}-\mathbf{r}_1)^2 \leq c_3/\gamma_1(\mathbf{r})$, where $\gamma_1(\mathbf{r})$ is the value obtained from Eq. (7) at $\mathbf{r}$. If the value of $\gamma_1(\mathbf{r}_1)$ is greater than $\gamma_1(\mathbf{r})$ for some $\mathbf{r}_1$ near $\mathbf{r}$, this argument suggests that $\gamma_1(\mathbf{r}_1)$ should be a better choice for the γ to be used in the evaluation of the wave function at $\mathbf{r}$. However, if $\gamma_1(\mathbf{r}_1)$ is so large that $(\mathbf{r}-\mathbf{r}_1)^2 > c_3/\gamma_1(\mathbf{r}_1)$, then the region of rapidly changing $C(\mathbf{s})$ is not near enough to $\mathbf{r}$ to contribute significantly to $\psi_E(\mathbf{r},\gamma)$ if $\gamma_1(\mathbf{r}_1)$ is used as the Gaussian width parameter at $\mathbf{r}$. Selecting a large width parameter at $\mathbf{r}$ on the basis of an estimate taken in a region that does not contribute significantly to the wave function at $\mathbf{r}$ would result in a larger than needed value of γ. In order to avoid this, the estimate $\gamma_1(\mathbf{r}_1)$ is replaced with $\min\{\gamma_1(\mathbf{r}_1), c_3/(\mathbf{r}-\mathbf{r}_1)^2\}$ when selecting the value of γ for the point $\mathbf{r}$. The value $c_3/(\mathbf{r}-\mathbf{r}_1)^2$ is used, since this is the largest value of γ for which the region of rapidly changing $C(\mathbf{s})$ is right at the edge of what is considered "near" to $\mathbf{r}$. Thus, a width parameter $\gamma_2(\mathbf{r}_1)=\min\{\gamma_1(\mathbf{r}_1), c_3/(\mathbf{r}-\mathbf{r}_1)^2\}$ is evaluated for each $\mathbf{r}_1$ for which $(\mathbf{r}-\mathbf{r}_1)^2 \leq c_3/\gamma_1(\mathbf{r})$, and the largest of these is selected as the value of γ to be employed in the calculation of the wave function at $\mathbf{r}$. A value of $c_3=2\hbar$ is used in all calculations in this work.

As mentioned above, the selection procedure for $\gamma(\mathbf{r})$ should not greatly increase the computational time for the GUWF. This rules out a complete calculation of the logarithmic derivative of C given by Eq. (6) for multidimensional problems, since this would include the calculation of $\partial^2 \mathbf{q}_t/\partial r_{0j}\partial r_{0k}$, where r_{0j} and r_{0k} are components of the initial position for the trajectory in directions perpendicular to the initial momentum. In order to avoid this, different n estimates of γ based on Eq. (7) are evaluated in an n-dimensional problem, rather than obtaining a single estimate by evaluating Eq. (6). The idea here is that if any of these estimates are large, then one or more of the $C^{-1}\partial C/\partial s_j$ are probably large, and a large value of γ should be employed. Of course, the justification for this rests on how well this works in practice.

The procedure employed in this work for multidimensional problems requires that each trajectory is run twice. A γ is chosen for each $\mathbf{r}$ the first time the trajectories are run, and then the $\psi_E(\mathbf{r},\gamma)$ is evaluated during the second run of the trajectories. When selecting the γ for $\mathbf{r}$, n estimates for γ are chosen for each trajectory that passes close to $\mathbf{r}$ using information obtained at the point of closest approach to $\mathbf{r}$ along

this trajectory, $\mathbf{r}_{ca}$. One estimate of γ is obtained using Eq. (7) with x_t taken to be the direction tangent to the trajectory r_{t1}. The other $n-1$ estimates are obtained using $F_j=(\partial\mathbf{r}_t/\partial r_{0j})\cdot(\partial\mathbf{q}_t/\partial\mathbf{r}_t)\cdot(\partial\mathbf{r}_t/\partial r_{0j})=(\partial\mathbf{r}_t/\partial r_{0j})\cdot(\partial\mathbf{q}_t/\partial r_{0j})$ for $\partial q_t/\partial x_t$ in Eq. (7) and $\partial F_j/\partial r_{t1}$ for $\partial^2 q_t/\partial x_t^2$ in Eq. (7), where $j=2,3,\ldots,n$ and $r_{0j}=s_j$. An alternative choice would have been to replace F_j with $F_j/|\partial\mathbf{r}_t/\partial r_{0j}|=\mathbf{e}_j\cdot(\partial\mathbf{q}_t/\partial r_{0j})$, where $\mathbf{e}_j=(\partial\mathbf{r}_t/\partial r_{0j})/|\partial\mathbf{r}_t/\partial r_{0j}|$. This change is not expected to alter the choice of γ significantly, although it might result in numerical problems at points where $|\partial\mathbf{r}_t/\partial r_{0j}|$ approaches zero. The possibility of $|\partial\mathbf{r}_t/\partial r_{0j}|$ approaching zero is the reason for adding c_2 in Eq. (7). A first estimate, γ_1, of the width parameter for the wave function at $\mathbf{r}$ from this trajectory is obtained from the largest of the n estimates of γ. The actual estimate from this trajectory is taken to be the $\min\{\gamma_1, c_3/(\mathbf{r}_{ca}-\mathbf{r})^2\}$. The rest of the selection procedure for the value of γ used in the calculation of the GUWF at $\mathbf{r}$ is identical to the one dimensional procedure.

F_j contains the derivative of $\mathbf{q}_t$ with respect to r_{0j}, while $\partial F_j/\partial r_{t1}$ is the derivative of this with respect to r_{t1}. This is employed in the calculations, as opposed to $\partial F_j/\partial r_{0k}$ for $k=2,3,\ldots,n$, because $\partial F_j/\partial r_{t1}$ is easily approximated numerically from information available along the trajectories by taking the difference of the values of F_j at the beginning and end of trajectory step containing the point of closet approach to $\mathbf{r}$ and dividing by the distance between these two trajectory points. Since F_j only contains $\partial\mathbf{p}_t/\partial r_{0j}$ and $\partial\mathbf{r}_t/\partial r_{0j}$, all the needed derivatives are already required for the fixed γ globally uniform and the primitive semiclassical calculations. In contrast, the evaluation of $\partial F_j/\partial r_{0k}$ would significantly increase the computational effort required. The estimate of γ from each trajectory that passes near $\mathbf{r}$ is obtained at the point of closest approach, rather than obtaining estimates at each point that is near to $\mathbf{r}$ in this trajectory and then selecting γ from this much larger set of estimates. This restriction is imposed because it significantly simplifies the procedure for choosing γ.
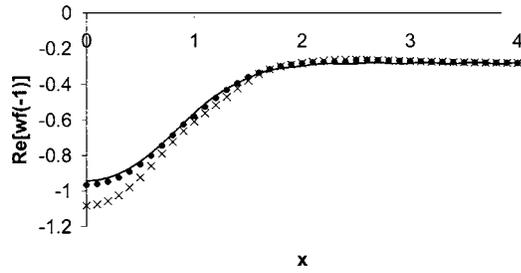
FIG. 3. The real part of $\psi(x,y)$ for $y=-1.0$, $E=1.3$ and $V(x,y)$ given by Eq. (8) with $m=80$ and $\hbar=1$, (——) quantum wave function, ($\times\times\times$) GUWF with $\gamma=1$, and ($\cdots$) variable γ GUWF.

III. NUMERICAL RESULTS

The globally uniform wave function employing an x dependent γ, chosen using Eq. (7), is compared with the quantum wave function for the one dimensional model problem with the potential given by Eq. (4) in Fig. 2. The use of the variable γ significantly improves the accuracy of the globally uniform wave function. As can be seen from Table I, the selected γ's reach as high as 32 near $x=0$, while the minimum value of $\gamma=1$ is chosen at larger values of $|x|$.

Now we consider the two dimensional scattering problem. The potential energy is

$$V(x,y) = e^{-(x^2+y^2)}, \tag{8}$$

with $\hbar=1$, a particle mass of $m=80$, and an energy of $E=1.3$. The incoming wave function is a plane wave

$$\psi_{\text{in}}(x,y) = e^{ip_0y/\hbar}, \tag{9}$$

where $p_0=(2mE)^{1/2}$. The quantum wave function is evaluated using a partial wave analysis.[22] The globally uniform wave functions are evaluated by running a set of trajectories. Each trajectory starts with the same value of y in the incoming asymptotic region and an initial momentum of p_0 in the y direction. The $s_1=t$ integration in Eq. (1) is performed numerically as each trajectory is run. The $s_2=x_0$ integration in Eq. (1) is performed numerically by selecting equally spaced values of $x_0=x(t)$ at $t=0$ for the trajectories. When the trajectories are run, the time dependent values of the stability matrix elements are integrated along with $\mathbf{r}$ and $\mathbf{p}$ by integrating the equations $\partial\mathbf{r}_t/\partial t=\mathbf{p}_t/m$, $\partial\mathbf{p}_t/\partial t=-\partial V(\mathbf{r}_t)/\partial\mathbf{r}$, $\partial\mathbf{M}_{rr}/\partial t=\mathbf{M}_{pr}/m$, and $\partial\mathbf{M}_{pr}/\partial t=-\partial^2V(\mathbf{r}_t)/\partial\mathbf{r}\partial\mathbf{r}\cdot\mathbf{M}_n/m$ using a fourth order Runge-Kutta routine, where $\mathbf{M}_{rr}=\partial\mathbf{r}_t/\partial\mathbf{r}_0$, and $\mathbf{M}_{pr}=\partial\mathbf{p}_t/\partial\mathbf{r}_0$.
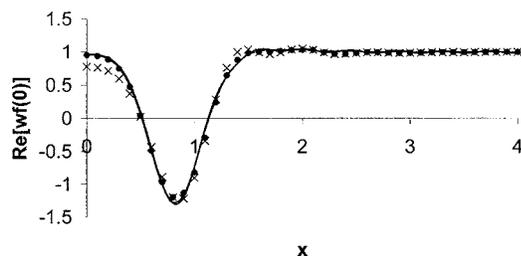

FIG. 4. The real part of $\psi(x,y)$ for $y=0.0$, $E=1.3$, and $V(x,y)$ given by Eq. (8) with $m=80$ and $\hbar=1$, (thick line) quantum wave function, (thin line) primitive, ($\times\times\times$) GUWF with $\gamma=1$, and ($\cdots$) variable γ GUWF.
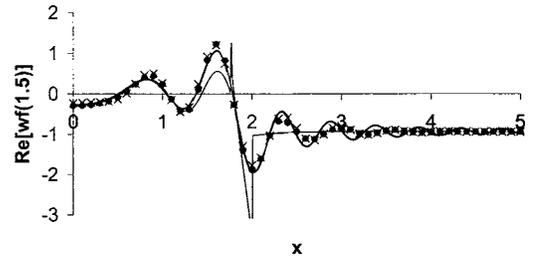

FIG. 5. The real part of $\psi(x,y)$ for $y=1.5$, $E=1.3$ and $V(x,y)$ given by Eq. (8) with $m=80$ and $\hbar=1$, (thick line) quantum wave function, (thin line) primitive, ($\times\times\times$) GUWF with $\gamma=1$, and ($\cdots$) variable γ GUWF.

The primitive wave function, which is given by Eq. (5) with $w_0=p_0y_0$, is evaluated by running a set of trajectories starting in the incoming asymptotic region at (x_0,y_0) with the appropriate momentum at closely spaced values of x_0. As each step in a trajectory is taken, it is checked whether any point $\mathbf{r}$ at which the wave function is to be evaluated falls between this trajectory and a corresponding step in the previous trajectory. The values of all the needed quantities to evaluate Eq. (5) are obtained by interpolating between the points nearest to $\mathbf{r}$ in the two consecutive trajectories. The number of caustics n_c is determined by counting the number of times $\det(\partial\mathbf{r}_t/\partial\mathbf{r}_0)$ changes sign along the trajectory.[23]

The real part of $\psi(x,y)$ is plotted in Figs. 3–6 as a function of x for fixed values of y. The results from quantum, primitive semiclassical, globally uniform with a fixed $\gamma=1$ and variable γ globally uniform calculations are compared. Figure 3 shows the results for $y=-1$. In this case, the incoming flux is interacting with $V(\mathbf{r})$ but has not reached the region of strongest interaction. In Fig. 4, $y=0$. This case corresponds to the region of largest potential. The classical trajectories have not yet experienced caustics for $y=-1$ and $y=0$. In these two cases, there is only one trajectory with the appropriate initial conditions that reaches each $\mathbf{r}=(x,y)$. Figures 5 and 6 correspond to $y=1.5$ and 3.5, respectively. In these cases, the trajectories have experienced caustics, and there is a range of x for which there are three trajectories that reach each $\mathbf{r}$. The selected values of γ for the variable γ globally uniform wave function are given in Table II. The data in the table show that γ is largest near $\mathbf{r}=0$ with a maximum value of 32, and it decreases to the minimum value of $\gamma=1$ as $\mathbf{r}$ increases.

For the $y=-1$ case, the globally uniform wave function with $\gamma=1$, while displaying the correct qualitative behavior, is less accurate in the region $0<x<1.5$, where the interac-
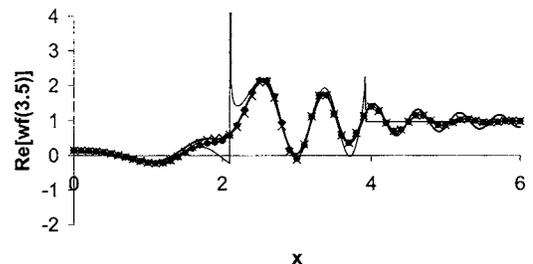

FIG. 6. The real part of $\psi(x,y)$ for $y=3.5$, $E=1.3$, and $V(x,y)$ given by Eq. (8) with $m=80$ and $\hbar=1$, (thick line) quantum wave function, (thin line) primitive, ($\times\times\times$) GUWF with $\gamma=1$, and ($\cdots$) variable γ GUWF.

TABLE II. The values of γ for the variable γ globally uniform wave function at various x and y for the two dimensional model problem.

x	$y=-1$	$y=0$	$y=1.5$	$y=3.5$
0.0	4	32	16	1
0.2	4	32	4	1
0.4	4	32	4	1
0.6	4	16	2	1
0.8	4	8	2	1
1.0	2	4	2	1
1.2	2	4	4	2
1.4	2	4	4	4
1.6	2	2	4	4
1.8	2	2	4	4
2.0	2	2	4	4
2.2	2	1	4	4
2.4	2	1	4	4
2.6	1	1	2	4
2.8	1	1	2	4
3.0	1	1	2	2
3.2	1	1	1	1
3.4	1	1	1	1

tion has significantly altered the phase of the wave function from the pure plane wave form of the incoming wave function. The use of a variable γ globally uniform wave function significantly improves the accuracy for the globally uniform wave function. The primitive wave function is not plotted in Fig. 3, since it is graphically indistinguishable from the quantum result for $y=-1$. The relatively small errors in the variable γ GUWF could be further reduced by choosing a larger value of c_1, which would result in larger γ's in this range of x, since this would result in the globally uniform wave function being closer to the primitive wave function.

Similar behavior is seen for the wave function at $y=0$. The GUWF with $\gamma=1$ has modest errors at small x. The use of a variable γ significantly reduces these errors, resulting in very good accuracy at all x. Once again the primitive wave function is very accurate over the entire range of x.

The situation changes significantly for larger y as can be seen from Figs. 5 and 6. The primitive wave function shows significant errors at all x much greater than 1, whereas the fixed γ globally uniform wave function provides a reasonably good approximation for the wave function. The primitive wave function has caustic singularities at about $x=1.8$ and $x=1.9$ for $y=1.5$ and near $x=2$ and $x=4$ for $y=3.5$. There is only one trajectory with the appropriate boundary conditions that reaches $\mathbf{r}$ for x larger than the x of the second caustic singularity. This trajectory starts with a large impact parameter x_0 and is only slightly deflected by the potential. For this reason, there is no interference between multiple trajectories in this range of x, and the primitive wave function does not display the decaying oscillations seen in the quantum wave function in this region. Oscillations are seen in the globally uniform wave function and the wave function is in good agreement with the quantum wave function through the first oscillation beyond the second caustic. At larger x, the oscillations decay more rapidly than in the quantum wave function and become out of phase with the quan-

tum oscillations. The use of a variable γ improves the accuracy of the globally uniform wave function compared with the fixed γ wave function for $x<1$ when $y=1.5$. Its value is very close to that of the fixed γ wave function in other regions for y equal to 1.5 and 3.5.

IV. DISCUSSION

This work explores the suggestion that, since the globally uniform wave function $\psi_E(\mathbf{r},\gamma)$ can be evaluated for any choice of γ as long as $\gamma>0$, it is reasonable to use the $\psi_E(\mathbf{r},\gamma)$ with a γ that is in some sense optimal for each point $\mathbf{r}$. Having noted this, the question becomes how to choose a good γ. A Monte Carlo sampling of the initial conditions for the classical trajectories is generally employed for many dimensional problems for semiclassical methods that require an integration over a set of classical trajectories. If a large γ is used, which corresponds to very narrow frozen Gaussian wave packets, then only trajectories that pass very near to a point $\mathbf{r}$ will contribute significantly to the wave function at that point. As a consequence a large γ necessitates a fine mesh of trajectories for accurate numerical results and this corresponds to a large Monte Carlo sample.

The prescription for the $\mathbf{r}$ dependent choice of γ employed in this work is motivated by the fact that the prefactor C in a semiclassical wave function $Ce^{f/\hbar}$ should be a slowly changing function compared with the exponential $e^{f/\hbar}$, since semiclassical methods are small $\hbar$ approximations. In the one and two dimensional model problems considered in this work, the primitive wave function is a very good approximation in some regions, but performs very badly in others, especially in regions near caustics. The GUWF with $\gamma=1$ at all $\mathbf{r}$ also has regions where it is very accurate and other regions where it has moderate errors. The variable γ GUWF, on the other hand, provides very good accuracy nearly everywhere for the model problems considered. The only significant deficiency in the variable γ GUWF results is the inability to accurately reproduce the oscillations in the wave function as x increases for positive y and x beyond the region of classical caustics.

We have taken the approach here that the width parameter γ should be kept as small as possible, since a large γ requires a finer mesh of trajectories. If this numerical consideration is ignored for the moment and only the accuracy of the GUWF is considered, it seems quite possible that a larger γ would produce a more accurate wave function in some regions and a small γ would do so in other regions. There are regions where the primitive wave function is highly accurate, and the $\gamma=1$ GUWF has noticeable errors. The GUWF approaches the primitive wave function in the large γ limit, suggesting that a relatively large γ is needed in these regions. The procedure presented for selecting γ chooses a fairly large γ in these regions, leading to a significant improvement in the accuracy of the GUWF. On the other hand, the primitive wave function provides a poor approximation to the quantum wave function in the region of caustics, while the $\gamma=1$ GUWF provides much better accuracy. In this region, a large γ would result in the GUWF approaching the poor quality of the primitive wave function. In general, the pro-

posed method for selecting γ does a good job of choosing a relatively large γ in regions where this is required to obtain accurate results and using a smaller γ in regions where a large γ should be avoided.

In this work, the constant c_1 in Eq. (7) is chosen to be $2\hbar$. This constant must have dimensions of action in order to make this equation dimensionally correct. The estimate for γ provided by Eq. (7) with this c_1 results in a $\gamma/\hbar$ that remains finite in the $\hbar \rightarrow 0$ limit. As a result, the width of the Gaussian packets does not go to zero in this limit. This occurs because the criterion used is that the relative changes in the prefactor are not large on the length scale of this width and the prefactor is independent of $\hbar$. However, as long as γ_{min} is independent of $\hbar$, the restriction that $\gamma \geqslant \gamma_{min}$ keeps γ from going to zero in the $\hbar \rightarrow 0$ limit.

The de Broglie wavelength provides another length scale in these problems that has not been considered in this work. An alternative criterion that could be used in the selection of γ is that the relative changes in the prefactor must be small over lengths on the scale of the de Broglie wavelength. In the examples considered in the work, the de Broglie wavelength is always less than unity, and this additional criterion would not alter the choice of γ. This might not be the case if a smaller mass is employed. In this case, using either the estimate for γ provided by the criterion employed in this work or the estimate provided by the de Broglie wavelength criterion, whichever is larger, in the selection of γ may result in improved accuracy.

While this paper has focused on the selection of an **r** dependent choice of γ in the application of the globally uniform wave function, the same argument can be made regarding the choice of γ in calculations of the Herman-Kluk (HK) propagator or other similar and more general semiclassical methods.[10–13] It has been shown that the GUWF and the HK propagator can be generalized to allow γ to be dependent on $\mathbf{r}_t$, $\mathbf{p}_t$, and t, and that the resulting wave function or propagator still satisfies the Schrödinger equation to first order in $\hbar$.[10] The suggestion here is that the γ value be selected for each **r**, the point at which the wave function or propagator is being evaluated, rather than selecting a γ for each $\mathbf{r}_t$, $\mathbf{p}_t$, and t along the trajectories being integrated. The argument is not that the resulting semiclassical quantity satisfies the Schrödinger equation to this order of $\hbar$, but rather that the

fixed γ GUWF or propagator satisfies the Schrödinger equation to this order for any value of γ, and it is reasonable to use a fixed γ wave function or propagator at each **r** that provides accurate results. It is worth noting that the criterion employed in this work for the selection of γ, or one similar to it, could also be applied in order to select a $\mathbf{r}_t$, $\mathbf{p}_t$, and t dependent γ, rather than an **r** dependent one. Additional study of this method on a wider range of numerical problems should provide greater insight concerning the choice of a good **r** dependent γ, further improving the implementation of the method.

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