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Uniform regularized semiclassical propogator for the 1/x^2 potential

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We apply recent methods for semiclassical time propagation involving non-Cartesian variables to the repulsive one-dimensional potential $V(x)=x^{-2}, x\geqslant 0$. In order to properly treat non-Cartesian variables, a quantum regularization is first performed which leads to a Langer-type potential correction term in the Gutzwiller–Van Vleck propagator. A nonuniform semiclassical treatment of $V(x)=x^{-2}$ using this regularization improves earlier unregularized results, and a uniform regularized propagator is very nearly exact for all times.

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I. REGULARIZED SEMICLASSICAL PROPAGATOR

A central result in semiclassical mechanics is the expression for the semiclassical approximation to the quantum propagator,

$$K(\mathbf{x}_b,\mathbf{x}_a,t)=\langle \mathbf{x}_b|e^{-i\hat{H}t/\hbar}|\mathbf{x}_a\rangle, \tag{1}$$

due to Van Vleck and Gutzwiller [1–3]:

$$K_{sc}(\mathbf{x}_b,\mathbf{x}_a,t)=(2\pi i\hbar)^{-n/2}\sum_r \sqrt{\left|\det\frac{\partial^2 R_r}{\partial \mathbf{x}_b \partial \mathbf{x}_a}\right|} \times\exp\left[\frac{iR_r(\mathbf{x}_b,\mathbf{x}_a,t)}{\hbar}-\frac{i\pi\mu_r}{2}\right]. \tag{2}$$

Equation (2) expresses the amplitude for getting from initial configuration $\mathbf{x}_a$ to final configuration $\mathbf{x}_b$ in time t under the action of time-independent Hamiltonian $\hat{H}$ as a sum over all *classical* trajectories r connecting $\mathbf{x}_a$ to $\mathbf{x}_b$ in time t. R_r is Hamilton's principal function for trajectory r, $R_r\equiv\int d\tau L(\mathbf{x},\dot{\mathbf{x}})$, while the term involving μ_r is a correction due to Gutzwiller that enables the earlier, short-time result of Van Vleck to be extended past the first conjugate point [2]; μ_r is the number of conjugate points encountered along trajectory r, i.e., the cumulative count over time of the number of zero eigenvalues of the matrix $\left(\frac{\partial^2 R}{\partial \mathbf{x}_b \partial \mathbf{x}_a}\right)^{-1}$.

Several studies have examined the difficulties arising in the derivation of the Gutzwiller–Van Vleck formula (2) when non-Cartesian variables are involved [4–6]; for one thing, the usual stationary phase approximation used in deriving the sum-over-trajectories formula [3] can fail when the variables $\mathbf{x}$ do not range from $-\infty$ to ∞.

We have recently given an approach to the semiclassical propagator for a class of one-dimensional (1D) systems with non-Cartesian variables x [5]. For the case where x is a single radial coordinate, $0\leqslant x\leqslant\infty$, we obtain a semiclassical propagator of a form very similar to (2). In this approach [5], we first perform a quantum regularization developed by Duru and Kleinert [4,7] which transforms the radial coordinate x to a Cartesian-like variable $\xi=\ln x$, $-\infty\leqslant\xi\leqslant\infty$, at the expense of introducing two additional integrations into the quantum propagator. Performing these integrals by stationary phase (consistent with the usual semiclassical approach [8]) and simplifying leads to our result for the regularized semiclassical propagator:

$$K_{sc}(\mathbf{x}_b,\mathbf{x}_a,t)=(2\pi i\hbar)^{-n/2}\sum_r \sqrt{\left|\det\frac{\partial^2 R'_r}{\partial \mathbf{x}_b \partial \mathbf{x}_a}\right|} \times\exp\left[\frac{iR'_r(\mathbf{x}_b,\mathbf{x}_a,t)}{\hbar}-\frac{i\pi\mu'_r}{2}\right]. \tag{3}$$

This expression is identical to the Gutzwiller–Van Vleck propagator (2), except that the classical quantities R_r and μ_r have been replaced by the analogous quantities for a *modified* classical system, in which an additional term ΔV is added to the potential energy function. (Full details of the derivation and the general form of the potential energy correction can be found in [5]; cf. also [4].)

An important application of our procedure is to systems with singular potentials $V(x)$ of the form C/x^α, $0<\alpha<2$. In this case the regularization leads to a potential correction term

$$\Delta V=\frac{\hbar^2}{8mx^2}, \tag{4}$$

the familiar Langer correction [9]. Langer's original derivation and use of this correction was in energy-domain computations [9]; our regularization procedure introduces the same correction into the time domain. Time-domain Langer corrections have previously been presented by an asymptotic analysis of the Bessel function in a partial wave expansion for the action [10–13]; however, this asymptotic analysis was later shown to be incorrect [4,14]. Gutzwiller ([2], Sec. 13.5) also provides a heuristic argument for using the Langer correction in the time domain.

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II. APPLICATION: $V(x)=1/x^2$

We now consider a one-dimensional system with repulsive potential $V(x)=1/x^2$, $0\leqslant x\leqslant\infty$. The propagator for this potential has previously been studied by Basile and Gray, who use a discretized WKB approximation to the semiclassical propagator which does not contain the regularization factor described above. Basile and Gray also develop a uniform WKB propagator for this potential, to handle trajectories which pass close to a caustic path [15]. The $1/x^2$ potential also has the advantage that the exact quantum propagator is known [15]:

$$K(x_b,x_a,t)=\frac{m\sqrt{x_b x_a}}{i\hbar t}\exp\left[\frac{im(x_b^2+x_a^2)}{2\hbar t}\right]I_\nu\left(\frac{mx_b x_a}{i\hbar t}\right). \quad (5)$$

The regularized semiclassical propagator (3) is expressed in terms of classical quantities determined for trajectories in the corrected potential

$$V(x)=\frac{1+\dfrac{\hbar^2}{8m}}{x^2}\equiv\frac{C}{x^2}. \quad (6)$$

We will first compare the nonuniform regularized semiclassical propagator to the unregularized results of Basile and Gray ($C=1$) and to the exact propagator (5). (Several approximations to the short-time propagator for the x^{-2} potential have been compared by Lolle *et al.* [16].)

A. Classical mechanics

1. Time of travel

The classical motion subject to the potential $V(x)=\dfrac{C}{x^2}$ is exactly soluble, through the basic energy equation

$$\dot{x}^2=\frac{2E}{m}-\frac{2C}{mx^2}. \quad (7)$$

Direct solution of this differential equation, for a trajectory going *directly* from x_a to $x_b>x_a$, gives the time of travel:

$$t=\frac{\sqrt{m}}{2E}\sqrt{2Ex^2-2C}\Big|_{x_a}^{x_b}. \quad (8)$$

For notational convenience, we define

$$A(x,E)\equiv\sqrt{2Ex^2-2C}. \quad (9)$$

Observe that $A=0$ at the inner turning point $x_{min}=\sqrt{C/E}$.

Now we characterize all trajectories in this system. There are two trajectories which connect x_a to x_b at a given energy E: a direct trajectory, and an indirect trajectory, which bounces off the potential wall (assuming both x_a and x_b are in the classically allowed region $x>\sqrt{C/E}$). We define

$$\gamma_a=-(\text{ sign of initial velocity}),$$

$$\gamma_b=(\text{ sign of final velocity}). \quad (10)$$

Using this notation and the basic solution for rightward motion (8), we can write the general time-of-travel formula:

$$t(x_b,x_a,E)=\gamma_a\frac{\sqrt{m}A(x_a,E)}{2E}+\gamma_b\frac{\sqrt{m}A(x_b,E)}{2E}$$
$$\equiv\gamma_a\frac{\sqrt{m}A_a}{2E}+\gamma_b\frac{\sqrt{m}A_b}{2E}. \quad (11)$$

We have introduced the shorthand $A_*\equiv A(x_*,E)$.

2. Hamilton's principal function

A similar direct integration of $R=\int L\,d\tau=\int(E-2V)\,d\tau$ gives Hamilton's principal function:

$$R(x_b,x_a,t)=Et-\gamma_a\sqrt{2Cm}\arccos\sqrt{\frac{C}{Ex_a^2}}$$
$$-\gamma_b\sqrt{2Cm}\arccos\sqrt{\frac{C}{Ex_b^2}}. \quad (12)$$

3. Density of trajectories

Next, we need the mixed second derivative of R, the density of trajectories. We use the standard result that $\partial R/\partial x_b|_{x_b,x_a,t}=p_b$ [2]:

$$\left.\frac{\partial^2 R}{\partial x_b\partial x_a}\right|_{x_b,x_a,t}=\frac{\partial p_b}{\partial x_a}=\sqrt{m}\gamma_b\frac{\partial}{\partial x_a}\sqrt{2E-\frac{2C}{x_b^2}}$$
$$=\frac{\gamma_b\sqrt{m}(\partial E/\partial x_a)}{\sqrt{2E-\dfrac{2C}{x_b^2}}}=\frac{\gamma_b\sqrt{m}x_b(\partial E/\partial x_a)}{A(x_b,E)}. \quad (13)$$

We compute $\partial E/\partial x_a$ by implicit differentiation of (11) with respect to x_a, holding x_b and t constant; some lengthy but straightforward computations lead to the result:

$$\frac{\partial^2 R}{\partial x_b\partial x_a}=\frac{-2E^2\sqrt{m}\gamma_a\gamma_b x_a x_b}{\gamma_a(2C-Ex_a^2)A_b+\gamma_b(2C-Ex_b^2)A_a}. \quad (14)$$

4. Conjugate points

We need to determine where $\partial^2 R/\partial x_b\partial x_a$ blows up; we define a function g, for which the following is true:

Lemma 1. For $x_a\neq x_{min}$,

$$\partial^2 R/\partial x_b \partial x_a \text{ blows up } \Leftrightarrow g(x_b,x_a,E) \equiv \frac{\gamma_a(2C-Ex_a^2)}{A_a} + \frac{\gamma_b(2C-Ex_b^2)}{A_b} = 0.$$

Proof: Since the denominator of $\partial^2 R/\partial x_b \partial x_a$ is $A_b A_a g(x_b,x_a,E)$, $g=0$ clearly implies that $\partial^2 R/\partial x_a \partial x_b$ blows up. On the other hand, if $\partial^2 R/\partial x_b \partial x_a$ blows up, can we have $g(x_b,x_a,E)\neq 0$? This would require $A_b=0$, so that $x_b^2=C/E$ and $2C-Ex_b^2\neq 0$. Hence, referring to (14), we would need $A_a=0$ in order for $\partial^2 R/\partial x_b \partial x_a$ to blow up. This, however, is not allowed by the hypothesis.

Computation of $\partial g(x_b,x_a,E)/\partial x_b$ shows that g always decreases along a trajectory: it starts from 0 at the beginning of the trajectory, decreases to $-\infty$ at the turning point if there is one, jumps to $+\infty$ just past the turning point, and decreases thereafter. Since conjugate points occur when $g=0$ (except at the initial instance $t=0$), we can conclude that the number of conjugate points, μ,

$$\mu = \begin{cases} 1 & \text{for indirect trajectories with } g(x_b,x_a,E)<0 \\ 0 & \text{otherwise.} \end{cases} \tag{15}$$

[This determination of conjugate point count also holds for the case $x_a=x_{min}$ (excluded in the hypothesis of the Lemma), as is clear from direct analysis of $\partial^2 R/\partial x_b \partial x_a$ when $x_a=x_{min}$.]

B. Expressing everything in terms of t

To this point, we have been computing all classical mechanical quantities as a function of energy E. However, to compute the regularized semiclassical propagator

$$K_{sc}(x_b,x_a,t) = \frac{1}{\sqrt{2\pi i\hbar}} \sum_{\substack{x_a \to x_b \\ \text{in time} t}} \left| \frac{\partial^2 R'}{\partial x_b \partial x_a} \right|^{\frac{1}{2}} \times \exp\left(\frac{iR'}{\hbar} - \frac{iM'\pi}{2} \right), \tag{16}$$

we must express everything in terms of t.

1. Inverting $t(E)$

Equation (11) gives $t(x_b,x_a,E)$, the time of travel for trajectories to get from x_a to x_b at energy E. To compute $K_{sc}(x_b,x_a,t)$, we need to find the trajectories which take time t to get from x_a to x_b. Hence, we need to find the energies E which make $t(x_b,x_a,E)$ equal a given time; that is, we must invert the function $t(x_b,x_a,E)$. This results in a quadratic equation in E, with the two solutions:

$$E = \frac{m(x_a^2+x_b^2) \pm 2\sqrt{m^2x_a^2x_b^2 - 2t^2Cm}}{2t^2}. \tag{17}$$

It is clear that t cannot exceed $t_F \equiv x_a x_b \sqrt{m/2C}$ (the notation is as in [15]); there are no trajectories at any energy which take longer than this to get from x_a to x_b.

2. Direct versus indirect trajectories

We have just found the energies (17) of the two trajectories which take time t to get from x_a to x_b; however, we still need to know if these trajectories are direct or indirect. To do this, we analyze the functions $t_{dir}(x_b,x_a,E)$ and $t_{ind}(x_b,x_a,E)$. A simple computation shows that

$$\frac{\partial t(x_b,x_a,E)}{\partial E} = \frac{g(x_b,x_a,E)}{2\sqrt{m}E^2}. \tag{18}$$

We have seen that for direct trajectories $g(x_b,x_a,E)<0$. Hence, $\partial t_{dir}/\partial E<0$. For indirect trajectories, $g(x_b,x_a,E)<0$ if and only if $x_b>x_{cp}(x_a,E)$, with $x_{cp}(x_a,E)$ the conjugate point to x_a at energy E. We thus need to find the relative positioning of x_b and $x_{cp}(x_a,E)$ for different energies E. We can determine $x_{cp}(x_a,E)$ explicitly by solving $g(x_{cp}(x_a,E),x_a,E)=0$ (recall that $\gamma_a=\gamma_b=1$ for indirect trajectories):

$$x_{cp}(x_a,E) = \frac{\sqrt{C}x_a}{\sqrt{Ex_a^2-C}}. \tag{19}$$

Clearly $x_{cp}(x_a,E)$ decreases as a function of E, and further analysis shows that $x_{cp}>x_b$ for the lowest allowed energy and $x_{cp}<x_b$ for the highest allowed energy. Thus, there is some energy $\tilde{E}$, so that $x_{cp}(E)>x_b$ for $E_{min}<E<\tilde{E}$, and $x_{cp}(E)<x_b$ for $\tilde{E}<E$. So, $g(x_b,x_a,E)>0$ for $E_{min}<E<\tilde{E}$, while $g(x_b,x_a,E)<0$ for $\tilde{E}<E$. Therefore, $\partial t/\partial E>0$ for $E_{min}<E<\tilde{E}$, while $\partial t/\partial E<0$ for $\tilde{E}<E$.

We now know the qualitative structure of $t_{dir}(x_b,x_a,E)$ and $t_{ind}(x_b,x_a,E)$ as functions of E. At $E=E_{min}$, when the smaller of x_a and x_b is on the potential wall, the direct and indirect paths collapse to the same path, so the functions t_{dir} and t_{ind} have the same value. We have seen that t_{dir} always decreases, whereas t_{ind} increases until $E=\tilde{E}$, then decreases thereafter. As $E\to\infty$, both functions approach 0, which is clear from (11) since $A(x,E)=O(\sqrt{E})$. Hence, the functions t_{dir} and t_{ind} are as shown in Fig. 1.

For a given value of t less than the critical value $t_F=x_a x_b\sqrt{m/2C}$ (the maximum value of t_{ind} in Fig. 1), we have seen that there are two energies E for which trajectories take time t to get from x_a to x_b. From Fig. 1, it is clear that for $t<t(x_b,x_a,E_{min})$, the larger E value is an indirect trajectory and the smaller E value is a direct trajectory. Similarly, for $t>t(x_b,x_a,E_{min})$, both trajectories are indirect.

Now, $t(x_b,x_a,E_{min})$ is travel time from the turning point $x_< \equiv \min(x_a,x_b)$ to $x_> \equiv \max(x_a,x_b)$, which is exactly what we found in (11) to be $\sqrt{m}A(x_>,E)/2E$:

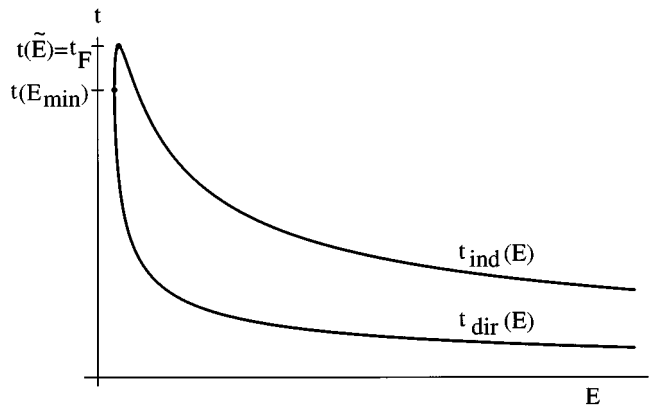

FIG. 1. Qualitative sketch of the graphs of $t_{dir}(E)$ and $t_{ind}(E)$ for motion in the potenital $V(x)=C/x^2$, $C>0$.

$$E_{min}=\frac{C}{x_<^2},$$

$$t(x_b,x_a,E_{min})=\frac{\sqrt{m}A(x_>,E_{min})}{2E_{min}}=\sqrt{\frac{m}{2C}}x_<\sqrt{x_>^2-x_<^2}. \tag{20}$$

3. A in terms of t

We can also get an expression for A_a,A_b in terms of (x_b,x_a,t), by directly transforming the definition of A into the variables (x_b,x_a,t):

$$A_*=\frac{|mx_*^2\pm\sqrt{m^2x_a^2x_b^2-2t^2Cm}|}{t\sqrt{m}}. \tag{21}$$

A sign analysis of the expression inside the absolute value, including the use of (20), leads to the expression

$$A_*=\gamma_*\frac{mx_*^2\pm\sqrt{m^2x_a^2x_b^2-2t^2Cm}}{\sqrt{m}t}\quad(*=a,b). \tag{22}$$

4. Conjugate points in terms of t

We now express g in terms of (x_b,x_a,t), by direct conversion to the variables (x_b,x_a,t) and subsequent simplification:

$$g=\frac{\mp 2E^2t^3\sqrt{m}\sqrt{m^2x_a^2x_b^2-2t^2Cm}}{(mx_a^2\pm\sqrt{m^2x_a^2x_b^2-2t^2Cm})(mx_b^2\pm\sqrt{m^2x_a^2x_b^2-2t^2Cm})}, \tag{23}$$

or the more condensed form:

$$g=\frac{\mp 2E^2t^3\sqrt{m^2x_a^2x_b^2-2t^2Cm}}{\gamma_a\gamma_bA_aA_bm^{3/2}t^2}=\frac{\mp 2\gamma_a\gamma_bE^2t\sqrt{m^2x_a^2x_b^2-2t^2Cm}}{m^{3/2}A_aA_b}. \tag{24}$$

For the top choice of signs (always indirect trajectories, by Sec. II B 2), $g<0$ by (23). For the bottom choice of signs, (24) shows that $g<0$ for direct trajectories ($\gamma_a\gamma_b=-1$) and $g>0$ for indirect trajectories ($\gamma_a\gamma_b=1$). Hence, using (15), we get a conjugate point for the top choice of sign, and not for the bottom. Thus, the index can be expressed as

$$e^{\frac{-i\pi\mu}{2}}=\exp\left(-\frac{i\pi}{4}\mp\frac{i\pi}{4}\right)=(i)^{-1/2}\exp\left(\mp\frac{i\pi}{4}\right). \tag{25}$$

5. Density in terms of t

We now rewrite the second derivative $\partial^2R/\partial x_a\partial x_b=-2E^2\sqrt{m}\gamma_a\gamma_bx_ax_b/A_aA_bg$ in terms of (x_b,x_a,t), using the relation (24) that $E^2\gamma_a\gamma_b/A_aA_bg=\mp m^{3/2}/2t\sqrt{m^2x_a^2x_b^2-2t^2Cm}$:

$$\frac{\partial^2R}{\partial x_a\partial x_b}=\frac{-2E^2\sqrt{m}\gamma_a\gamma_bx_ax_b}{A_aA_bg}=\frac{\pm m^2x_ax_b}{t\sqrt{m^2x_a^2x_b^2-2t^2Cm}}. \tag{26}$$

6. Hamilton's principal function in terms of t

Recall from (12) that

$$R=Et-\gamma_a\sqrt{2Cm}\arccos\sqrt{\frac{C}{Ex_a^2}}+\gamma_b\sqrt{2Cm}\arccos\sqrt{\frac{C}{Ex_b^2}}$$

$$=Et-\gamma_a\sqrt{2Cm}\left(\arccos\sqrt{\frac{C}{Ex_a^2}}+\frac{\gamma_b}{\gamma_a}\arccos\sqrt{\frac{C}{Ex_b^2}}\right).$$

If arccos represents the multivalued inverse cosine function, then

$$\arccos X\pm\arccos Y=\arccos[XY\mp\sqrt{(1-X^2)(1-Y^2)}]. \tag{27}$$

Analysis of the relative sizes of $X=\sqrt{C/Ex_a^2}$ and $Y=\sqrt{C/Ex_b^2}$, and the sign of $XY\mp\sqrt{(1-X^2)(1-Y^2)}$ leads to a similar relation for the single valued arccos functions:

$$\arccos X\pm\arccos Y=\gamma_a\arccos(XY\mp\sqrt{1-X^2}\sqrt{1-Y^2}). \quad (28)$$

We directly compute and simplify to find

$$XY\mp\sqrt{(1-X^2)(1-Y^2)} = \mp\sqrt{m^2x_a^2x_b^2-2Cmt^2}\frac{1}{mx_ax_b}. \quad (29)$$

Finally, we can express Hamilton's principal function in terms of (x_b,x_a,t):

$$R=\frac{m(x_a^2+x_b^2)\pm 2\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{2t}-\sqrt{2Cm}\left(\frac{\pi}{2}\pm\frac{\pi}{2}\mp\arccos\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{mx_ax_b}\right). \quad (30)$$

C. Assembling the regularized semiclassical propagator K_{sc}

Now we are ready to evaluate the semiclassical propagator (16), with the sum involving two trajectories. The amplitude $1/\sqrt{2\pi i\hbar|\partial^2R'/\partial x_a\partial x_b|}^{1/2}$ is the same for the two trajectories taking time t. Each term $iR'/\hbar-i\pi M'/2$ in the exponent which does not have a $\pm$ or a $\mp$ will survive as is, while those which do will become part of a cos term:

$$K=\sqrt{\frac{2x_ax_b}{\pi\hbar t}}\frac{m(m^2x_a^2x_b^2-2Cmt^2)^{-1/4}}{i}\exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t}-\frac{i\pi\sqrt{2Cm}}{2\hbar}\right]\cos\left[\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{\hbar t}-\frac{\pi\sqrt{2Cm}}{2\hbar}+\frac{\sqrt{2Cm}}{\hbar}\arccos\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{mx_ax_b}-\frac{\pi}{4}\right]$$

$$=\frac{1}{i}\sqrt{\frac{2m}{\pi\hbar t}}\left(1-\frac{t^2}{t_F^2}\right)^{-1/4}\exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t}-\frac{i\pi\sqrt{2Cm}}{2\hbar}\right]\cos\left[\frac{\sqrt{2Cm}\sqrt{\frac{t_F^2}{t^2}-1}}{\hbar}-\frac{\pi\sqrt{2Cm}}{2\hbar}+\frac{\sqrt{2Cm}}{\hbar}\arccos\sqrt{1-\frac{t^2}{t_F^2}}-\frac{\pi}{4}\right]. \quad (31)$$

(for $t<t_F=\sqrt{m}x_ax_b/\sqrt{2C}$). In Figs. 2 and 3, we plot the unregularized ($C=1$) and regularized ($C=1+\hbar^2/8,\hbar=1$) semiclassical propagators together with the exact propagator (5).

Not surprisingly, the semiclassical expressions fail near the caustic time $t=t_F$, since the two time-t trajectories (stationary points in path space) coalesce at $t=t_F$. The uniform semiclassical computation in the next section will remove this difficulty. For now, however, we note for $t\ll t_F$, when we expect the primitive semiclassical approximation to apply, the regularized computation provides a small but clear improvement to the unregularized approach.

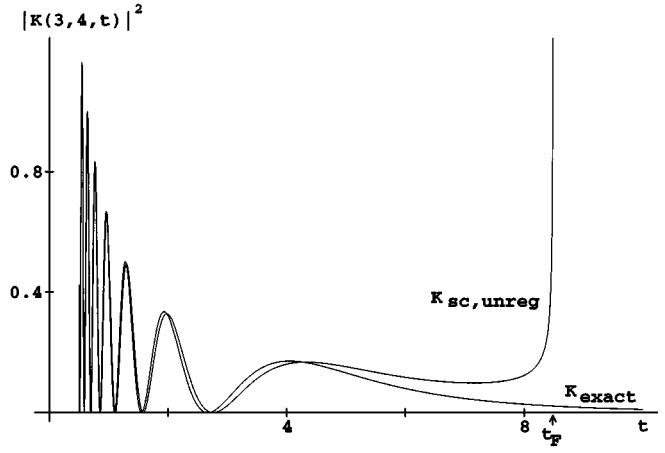

FIG. 2. Comparison of the unregularized semiclassical propagator $K(3,4,t)$ to the exact propagator for $V(x)=1/x^2$.

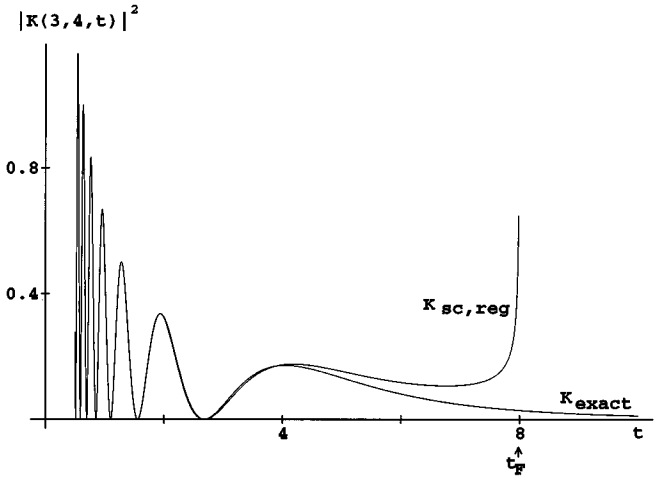

FIG. 3. Comparison of the regularized semiclassical propagator $K(3,4,t)$ to the exact propagator for $V(x)=1/x^2$.

III. UNIFORM SEMICLASSICAL APPROXIMATION

In this section we extend our regularized semiclassical treatment to a uniform approach able to treat the whole range of propagation times: $t<t_F$, $t\simeq t_F$, and $t>t_F$. The underlying classical mechanics is, of course, the same, as expressed in Eqs. (25), (26), and (30).

Uniform approximations were developed to handle coalescence of stationary points in the stationary phase approximation [17], and have thus played an important role in the development of semiclassical methods, since the stationary paths in the Gutzwiller–VanVleck sum will coalesce for certain travel times [3,18,19]. Important recent studies of uniform time-domain propagators have been made by Basile and Gray [15] and Campolieti and Brumer [20]. We now apply these results to the regularized $1/x^2$ potential under study.

A. Classically allowed region

In the classically allowed region, there are exactly two real trajectories connecting two points in a given travel time $t<t_F$; these coalesce to a single trajectory at $t=t_F$ and then disappear, the standard and simplest setting for a uniform treatment. The nonuniform stationary phase treatment uses a quadratic approximation to Hamilton's principal function R at each stationary path (classical trajectory); here we instead consider both stationary points at once by mapping R onto a cubic polynomial $R=1/3\,u^3-\gamma u+A$ [17,18]. The parameters γ and A change with the time of travel so that the stationary points coalesce at $t=t_F$ as required. Asymptotic evaluation of the discretized path integral under this cubic mapping provides the uniform semiclassical propagator (cf. [18,20]):

$$K(x_b,x_a,t)=(2\pi i\hbar)^{-1/2}\left\{\left|\frac{\partial^2 R}{\partial x_a\partial x_b}\right|_{(1)}^{1/2}\times Bi^{(-)}(-\gamma)\exp\left[\frac{iR_{(1)}}{\hbar}-\frac{i\pi M_{(1)}}{2}\right]+\left|\frac{\partial^2 R}{\partial x_a\partial x_b}\right|_{(2)}^{1/2}\times Bi^{(+)}(-\gamma)\exp\left[\frac{iR_{(2)}}{\hbar}-\frac{i\pi M_{(2)}}{2}\right]\right\},\tag{32}$$

where

$$Bi^{(\pm)}(-\gamma)\equiv\sqrt{\pi}[\,\gamma^{1/4}\mathrm{Ai}(-\gamma)\pm i\,\gamma^{-1/4}\mathrm{Ai}'(-\gamma)]\times\exp\left[\mp i\left(\frac{2}{3}\,\gamma^{3/2}-\frac{\pi}{4}\right)\right]\tag{33}$$

and

$$\gamma\equiv\left(\frac{3(R^{(2)}-R^{(1)})}{4\hbar}\right)^{2/3}.\tag{34}$$

The function Ai is the Airy function. The trajectory labeled by (1) is the one with the smaller value of R [15]. Hence, we must determine which classical trajectory gives the smaller value of R.

It will be convenient to rewrite R by noting that

$$\frac{\pi}{2}-\arccos\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{mx_ax_b}=\arctan\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{t\sqrt{2Cm}}\tag{35}$$

as a simple triangle diagram will demonstrate. If we define

$$X\equiv\frac{\sqrt{m^2x_a^2x_b^2-2Cmt^2}}{t\sqrt{2Cm}}\tag{36}$$

then R is given by

$$R=\frac{m(x_a^2+x_b^2)}{2t}\pm\sqrt{2Cm}X-\sqrt{2Cm}\left(\frac{\pi}{2}\pm\arctan X\right)=\frac{m(x_a^2+x_b^2)}{2t}-\sqrt{2Cm}\frac{\pi}{2}\pm\sqrt{2Cm}(X-\arctan X).\tag{37}$$

It is easily shown that $f(X)\equiv X-\arctan X>0$ for $X>0$; hence, the top choice of signs has the larger value of R.

Furthermore, from this computation, we can write γ as

$$\gamma=\left(\frac{3\sqrt{2Cm}(X-\arctan X)}{2\hbar}\right)^{2/3}.\tag{38}$$

Thus, the term $\exp[\mp 2/3\,i\gamma^{3/2}]$ in the functions Bi equals:

$$\exp\left[\mp\frac{2}{3}i\,\gamma^{3/2}\right]=\exp\left[\mp\frac{i\sqrt{2Cm}(X-\arctan X)}{\hbar}\right]\tag{39}$$

and cancels the $\pm$ term in $\exp[iR^{(\,)}/\hbar]$[cf. (37)]. In addition, the term $\exp[\pm i\pi/4]$ in the functions Bi cancels the term $\exp[-i\pi\mu^{(\,)}/2]$, except for the leading term $(i)^{-1/2}$[cf. (25)].

We can now write a compact expression for the uniform semiclassical propagator (32), pulling out of the braces the absolute value of the second derivative and the non-$\pm$ part of R, which are the same for the two trajectories:

$$K_u(x_b,x_a,t)=(2i\hbar)^{-\frac{1}{2}}(i)^{-\frac{1}{2}}\exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t}-\frac{i\sqrt{2Cm}\,\pi}{2\hbar}\right]\left|\times\frac{\partial^2 R}{\partial x_a\partial x_b}\right|_{(\,)}^{\frac{1}{2}}\{[\,\gamma^{\frac{1}{4}}\mathrm{Ai}(-\gamma)-i\,\gamma^{-\frac{1}{4}}\mathrm{Ai}'(-\gamma)]+[\,\gamma^{\frac{1}{4}}\mathrm{Ai}(-\gamma)+i\,\gamma^{-\frac{1}{4}}\mathrm{Ai}'(-\gamma)]\},$$
$$=2\,\gamma^{\frac{1}{4}}\mathrm{Ai}(-\gamma)\,\frac{1}{i\sqrt{2\hbar}}\exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t}-\frac{i\sqrt{2Cm}\,\pi}{2\hbar}\right]\left|\frac{\partial^2 R}{\partial x_a\partial x_b}\right|_{(\,)}^{\frac{1}{2}}.\tag{40}$$

We now insert the fact that

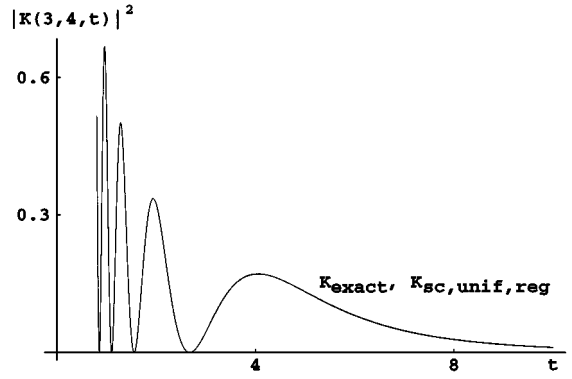

FIG. 4. Comparison of the regularized uniform propagator $K(3,4,t)$ to the exact propagator for $V(x)=1/x^2$.

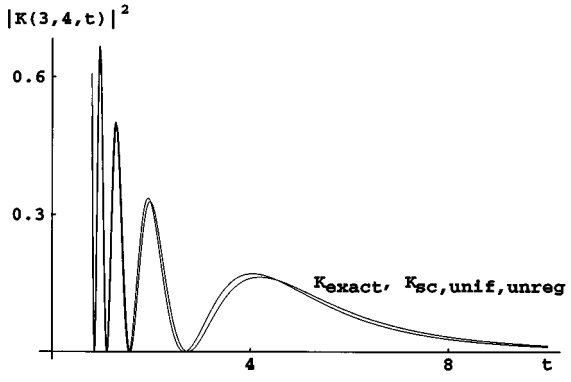

FIG. 5. Comparison of the unregularized uniform propagator $K(3,4,t)$ to the exact propagator for $V(x)=1/x^2$.

$$\left|\frac{\partial^2 R}{\partial x_b \partial x_a}\right|_{()} = \frac{m^2 x_a x_b}{X t^2 \sqrt{2Cm}}$$

to find that

$$K_u(x_b,x_a,t) = \frac{m\sqrt{2x_a x_b}}{it\sqrt{X\hbar}(2Cm)^{1/4}}\gamma^{1/4}\mathrm{Ai}(-\gamma) \times \exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t} - \frac{i\sqrt{2Cm}\pi}{2\hbar}\right]. \quad (41)$$

B. Classically disallowed region

We now analytically continue this expression into the region where there are no real classical trajectories, and find that everything carries through without difficulty. We consider two disallowed trajectories which are the analytic continuation of the two trajectories from the allowed region; we thus use the same classical mechanical formulas (25), (26), and (30).

Now the quantity X switches from being real and positive to being pure imaginary (we will take it with positive imaginary part). In addition, arctan$X$ will also be pure imaginary ($\tan z = e^{iz}-e^{-iz}/i(e^{iz}+e^{-iz})$ is pure imaginary when z is pure imaginary). Hence, the expression for γ is a pure imaginary number to the 2/3 power, which will be real and negative [15].

The remaining derivation of the uniform semiclassical propagator goes through as before, giving the same result. We must take care to treat the terms $\sqrt{X}$ and $\gamma^{1/4}$ correctly, taking the principal value in each. Since X is pure imaginary with positive imaginary part and γ is real and negative, each of these expressions will have argument $\pi/4$, and hence the arguments will cancel in the uniform propagator. Hence, without loss of generality, we may write $|X|$ and $|\gamma|$ in the formula for K_u and unambiguously cover both the allowed and disallowed regions (cf. [15]):

$$K_u(x_b,x_a,t) = \frac{m\sqrt{2x_a x_b}\,|\gamma|^{1/4}\mathrm{Ai}(-\gamma)}{it\sqrt{\hbar|X|}(2Cm)^{1/4}} \times \exp\left[\frac{im(x_a^2+x_b^2)}{2\hbar t} - \frac{i\sqrt{2Cm}\pi}{2\hbar}\right]. \quad (42)$$

The comparison between this regularized uniform approximation ($C=1+\hbar^2/8, \hbar=1$) and the exact result is very good for this system; as Fig. 4 shows, the propagators are indistinguishable to the naked eye. Basile and Gray [15] compared the unregularized uniform propagator to the exact propagator for this system; this comparison is recreated in Fig. 5 by inserting $C=1$ into K_u. Figure 6 shows that the regularized uniform approximation is not in fact exact for this system, with an error of about 0.5%.

IV. CONCLUSION

We have applied a semiclassical regularization to evaluate the propagator for the potential $V(x)=1/x^2$, with non-Cartesian coordinate $x \geq 0$; this regularization introduces a Langer-type correction term to the potential, which can then be treated with standard semiclassical methods. In the case studied here of a repulsive potential, classical trajectories in the unregularized system do not reach the problematic edge of the variable definition ($x=0$), so that one might think

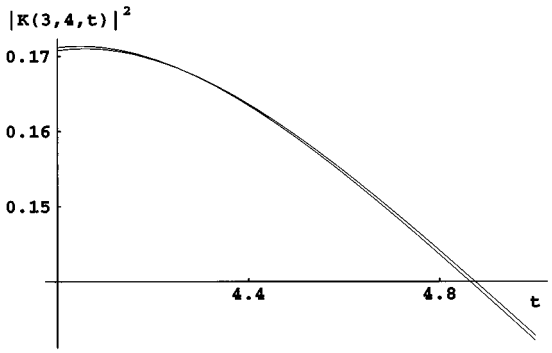

FIG. 6. Closer look at the comparison of the regularized uniform propagator $K(3,4,t)$ to the exact propagator for $V(x)=1/x^2$.

regularization to be unnecessary. However, we have demonstrated that, for the $1/x^2$ system, regularization results in a small but clear improvement to the accuracy of the semiclassical propagator. In fact, when a uniform treatment is combined with this regularization technique, the semiclassical propagator for $V(x)=1/x^2$ is very nearly exact. We note that, in the case of an attractive potential such as $V(x)=-1/x, x\geqslant 0$, regularization affects the qualitative nature of the classical trajectories (keeping them away from the singularity at $x=0$ with which they collide in the unregularized system), and thus plays a more important role in the computation of the semiclassical propagator (cf. [5]). Thus, in studying systems with non-Cartesian coordinates or singular potentials semiclassically, the regularization procedure applied here should be invoked.

ACKNOWLEDGMENT

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[1] J.H. Van Vleck, Proc. Natl. Acad. Sci. **14**, 178 (1928).
[2] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, Berlin, 1990).
[3] M.V. Berry and K.E. Mount, Rep. Prog. Phys. **35**, 315 (1972).
[4] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics* (World Scientific, Singapore, 1990).
[5] R.S. Manning and G.S. Ezra, Phys. Rev. A **50**, 954 (1994).
[6] R.S. Manning, Ph.D. thesis, Cornell University, 1994 (unpublished).
[7] I.H. Duru and H. Kleinert, Phys. Lett. B **84**, 185 (1979).
[8] W.H. Miller, Adv. Chem. Phys. **25**, 69 (1974).
[9] R.E. Langer, Phys. Rev. **51**, 669 (1937).
[10] D. Peak and A. Inomata, J. Math. Phys. **10**, 1422 (1969).
[11] C.C. Gerry and A. Inomata, Phys. Lett. A **84**, 172 (1981).
[12] F. Steiner, Phys. Lett. A **106**, 356 (1984).
[13] F. Steiner, Phys. Lett. A **106**, 363 (1984).
[14] F. Steiner, in *Path Integrals from meV to MeV*, edited by M.C. Gutzwiller (World Scientific, Singapore, 1986).
[15] A.G. Basile and C.G. Gray, J. Comput. Phys. **101**, 80 (1992).
[16] L.I. Lolle, C.G. Gray, J.D. Poll, and A.G. Basile, Chem. Phys. Lett. **177**, 64 (1991).
[17] C. Chester, B. Friedman, and F. Ursell, Proc. Cambridge Philos. Soc. **53**, 599 (1957).
[18] J.N.L. Connor, Mol. Phys. **25**, 181 (1973).
[19] L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
[20] G. Campolieti and P. Brumer, Phys. Rev. A **50**, 997 (1994).