

## Semiclassical calculation of off-shell $T$ -matrix elements

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A semiclassical approximation to the off-shell  $T$ -matrix elements  $t_i(p, p'; E)$  for potential scattering is derived for the case of local potentials. The approximation satisfies the off-shell unitarity relation. The advantage of the semiclassical description is twofold: It permits fast numerical calculations and allows also a classical understanding of the matrix elements. Classically allowed (oscillatory) and classically forbidden (exponentially damped) regions in the  $p, p'$  plane are discussed. Numerical examples are presented for purely repulsive potentials.

### I. INTRODUCTION

Inelastic or reactive scattering of three or more particles can be conveniently described by equations, which are completely based on the off-shell matrix elements of the two-body  $T$  operator. Exact equations like the Faddeev equations for three-particle scattering<sup>1</sup> or approximation schemes like the multiple-scattering expansion<sup>2</sup> or the impulse approximation<sup>3</sup> are of this type. Therefore, an understanding and an effective calculation method of the  $T$ -matrix elements is very important for an understanding and a solution of problems involving three or more particles.

Considerable effort has been devoted to the calculation of off-shell  $T$ -matrix elements: For the Coulomb potential the matrix elements are known<sup>4</sup> and for a few other potentials the  $s$ -wave part has been obtained in closed form.<sup>5</sup> An analytical expression for potentials consisting of a chain of rectangular wells has been given by Van Leeuwen and Reiner<sup>6</sup> and for arbitrary local potentials an effective calculation method based on this work has been presented recently.<sup>7,8</sup> Approximate methods are rather rare and confined to variational-type calculations,<sup>9</sup> which do not naturally lead to an "understanding" of the matrix elements, and to a Glauber approximation to the full  $T$  matrix without an angular-momentum decomposition.<sup>10</sup>

The semiclassical approximation derived in the present paper is assumed to meet two requirements: The derived formula is a reliable and easily applicable approximation and allows also an interpretation in terms of classical paths. It may therefore lead to a better insight not only into the two-body but also the three-body problem.

The general semiclassical theory, i.e., the limiting case of quantum mechanics, when  $\hbar$  is small compared with the classical action functions, is one of the most successful approxima-

tion schemes in atomic scattering.<sup>11</sup> A detailed discussion of this approximation can be found in the excellent reviews by Miller<sup>12</sup> and by Berry and Mount.<sup>13</sup> The semiclassical theory has a close connection with the principles of ray optics: the "rays" in semiclassical scattering are the classical trajectories. The phase is determined by the classical action along the path and the intensity by the density of paths. The superposition of several contributing paths gives rise to an interference structure in the classically allowed regions. During the last years the idea of complex-valued classical trajectories for classically forbidden processes has been developed and successfully applied to a variety of problems.<sup>12,14</sup> Complex-valued trajectories will also appear in the semiclassical approximation to the  $T$  matrix.

Section II gives the basic formulas for the  $T$  matrix. In Sec. III the semiclassical approximation to the  $T$  matrix is derived and a few numerical sample calculations are presented. Comments and conclusions appear in Sec. IV.

### II. GENERAL THEORY

In this section we give a brief outline of the well-known  $T$  matrix formalism. The  $T$  operator for potential scattering is defined by

$$T(E) = V + V(E - H_0)^{-1}T(E). \quad (1)$$

Here  $H_0$  is the kinetic energy operator and  $V$  is the potential, which is assumed to be local and spherically symmetric. The energy  $E$  is allowed to be complex. For positive real  $E$  the limit  $E + i\epsilon$ ,  $\epsilon \rightarrow 0$  ( $\epsilon > 0$ ) is understood.

We are interested in the calculation of the matrix elements of  $T$  in momentum space  $\langle \vec{p} | T(E) | \vec{p}' \rangle$ , where the momenta are allowed to be off-shell, i.e., they may differ from  $p_E = (2mE)^{1/2}$  ( $m$  is the reduced mass). It should be recalled, that the on-shell matrix elements (i.e.,  $|\vec{p}| = |\vec{p}'| = p_E$ ) are directly related to the differential cross section by

$$\frac{d\sigma}{d\Omega}(\vec{p}-\vec{p}') = |-4\pi^2 m\hbar \langle \vec{p} | T(E) | \vec{p}' \rangle|^2, \quad (2)$$

with the normalization  $\langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p}-\vec{p}')$ . The usual partial-wave expansion

$$\langle \vec{p} | T(E) | \vec{p}' \rangle = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) t_l(p, p'; E) P_l(\hat{p} \cdot \hat{p}') \quad (3)$$

defines the partial-wave matrix elements  $t_l(p, p'; E)$  ( $p = |\vec{p}|$ ,  $p' = |\vec{p}'|$ ), which can be written

$$t_l(p, p'; E) = \frac{2}{\pi\hbar p p'} \int_0^{\infty} \hat{j}_l(p r/\hbar) V(r) \omega_l(r, p'; E) dr, \quad (4)$$

where  $\hat{j}_l$  is the Riccati-Bessel function.<sup>15</sup> The "off-shell wave function"  $\omega_l(r, p; E)$  is a solution of the inhomogeneous differential equation<sup>6-8</sup>

$$\left( \hbar^2 \frac{d^2}{dr^2} - \frac{\hbar^2 l(l+1)}{r^2} + 2m[E - V(r)] \right) \omega_l(r, p; E) = (p_E^2 - p^2) \hat{j}_l(p r/\hbar). \quad (5)$$

This equation reduces to the well-known Schrödinger equation for  $p = p_E$ . The  $\omega_l(r, p; E)$  are the coefficients of the partial-wave expansion of the Møller operator  $\Omega$ , which is defined by

$$T(E) = V\Omega(E), \quad (6)$$

in a mixed coordinate-momentum representation<sup>6-8</sup>:

$$\begin{aligned} \langle \vec{r} | \Omega(E) | \vec{p} \rangle &= \frac{1}{(8\pi^3 \hbar)^{1/2} p r} \\ &\times \sum_{l=0}^{\infty} i^l (2l+1) \omega_l(r, p; E) P_l(\hat{r} \cdot \hat{p}). \end{aligned} \quad (7)$$

The off-shell wave function  $\omega_l(r, p; E)$  satisfies the boundary condition

$$\omega_l(r, p; E) \xrightarrow{r \rightarrow \infty} \hat{j}_l(p r/\hbar) - \pi m p t_l(p, p_E; E) \hat{h}_l^*(p_E r/\hbar), \quad (8)$$

where  $\hat{h}_l^*$  is the Riccati-Hankel function.<sup>15</sup> Equation (8) is easily derived in direct analogy to the usual derivation of the on-shell asymptotic of the solution of the Schrödinger equation<sup>16</sup>

$$\begin{aligned} \omega_l(r, p_E; E) &\xrightarrow{r \rightarrow \infty} \hat{j}_l(p_E r/\hbar) \\ &- \pi m p_E t_l(p_E, p_E; E) \hat{h}_l^*(p_E r/\hbar) \\ &\xrightarrow{r \rightarrow \infty} e^{i\eta_l} \sin\left(\frac{p_E r}{\hbar} - l\frac{\pi}{2} + \eta_l\right), \end{aligned} \quad (9)$$

which is the on-shell version of Eq. (8).

In the following some useful properties of the

$T$ -matrix elements are listed, which should be satisfied by a reasonable approximation. The energy  $E$  is assumed to be real and positive.

(a) The scattering phase shifts  $\eta_l$  are connected with the on-shell  $T$ -matrix elements by

$$t_l(p_E, p_E; E) = -(1/\pi m p_E) e^{i\eta_l} \sin\eta_l. \quad (10)$$

(b) The  $T$ -matrix elements are symmetric:

$$t_l(p', p; E) = t_l(p, p'; E). \quad (11)$$

(c) The half-shell quantity

$$\phi_l(p, p_E) = e^{-i\eta_l} t_l(p, p_E; E), \quad (12)$$

which was introduced by Baranger *et al.*,<sup>17</sup> is real.

(d) The most important equation is the off-shell unitarity relation, which is

$$\text{Im} t_l(p, p'; E) = -\pi m p_E \phi_l(p, p_E) \phi_l(p', p_E), \quad (13)$$

in terms of the  $\phi_l(p, p_E)$ ; i.e., the imaginary part of the off-shell  $T$  matrix is determined by half-shell quantities.

### III. SEMICLASSICAL APPROXIMATION

In our semiclassical approximation we follow the formal development outlined in Sec. II. First we obtain a semiclassical (i.e., WKB-type) approximation to the off-shell wave function  $\omega_l(r, p; E)$ . The second step is the asymptotic ( $\hbar \rightarrow 0$ ) evaluation of the integral (4) using the method of stationary phase. The resulting expression for the  $t_l(p, p'; E)$  is then interpreted in terms of classical paths. The energy is assumed to be real and positive.

#### A. On-shell and half-shell $T$ -matrix elements

The semiclassical approximation to the on-shell  $T$  matrix is easily obtained by inserting the WKB phase shift

$$\eta_l = \frac{1}{\hbar} \int_{r_0}^{\infty} [p_l(r) - p_E] dr - \frac{p_E r_0}{\hbar} + \left(l + \frac{1}{2}\right) \frac{\pi}{2}, \quad (14)$$

with the radial momentum

$$p_l(r) = [p_E^2 - 2mV(r) - L^2/r^2]^{1/2} \quad (15)$$

and the classical angular momentum

$$L = (l + \frac{1}{2})\hbar \quad (16)$$

into Eq. (10).  $r_0$  is the classical turning point. In view of what follows we note here the well-known WKB wave function belonging to the boundary condition  $\sin(p_E r/\hbar - \frac{1}{2} l\pi + \eta_l)$  at infinity:

$$\psi_i^{(1)}(r) = \left( \frac{p_E}{|p_i(r)|} \right)^{1/2} \begin{cases} \frac{1}{2} \exp\left(\frac{1}{\hbar} \int_{r_0}^r |p_i(r')| dr'\right), & r < r_0, \\ \sin\left(\frac{1}{\hbar} \int_{r_0}^r p_i(r') dr' + \frac{\pi}{4}\right), & r > r_0. \end{cases} \quad (17a)$$

$\psi^{(1)}$  is exponentially decreasing in the forbidden region  $r < r_0$ . We also need the WKB wave function belonging to the outgoing boundary condition  $\exp(i(p_E r/\hbar - \frac{1}{2} l\pi + \eta_l))$  at infinity

$$\psi_i^{(2)}(r) = \left( \frac{p_E}{|p_i(r)|} \right)^{1/2} \begin{cases} \exp\left(-\frac{1}{\hbar} \int_{r_0}^r |p_i(r')| dr'\right) + \frac{i}{2} \exp\left(\frac{1}{\hbar} \int_{r_0}^r |p_i(r')| dr'\right), & r < r_0, \\ \exp\left[i\left(\frac{1}{\hbar} \int_{r_0}^r p_i(r') dr' + \frac{\pi}{4}\right)\right], & r > r_0. \end{cases} \quad (17b)$$

In the half-shell case ( $p' = p_E$ )  $\omega_i$  is identical with the usual radial wave function, which is approximated by the WKB wave function with the correct normalization of Eq. (9):

$$\omega_i(r, p_E; E) = e^{i\eta_l} \psi_i^{(1)}(r). \quad (18)$$

We further use the asymptotic form of the Riccati-Bessel function for large values of index and argument<sup>19</sup>

$$\hat{j}_l\left(\frac{pr}{\hbar}\right) = \frac{1}{(\sin\beta)^{1/2}} \cos\left[\left(l + \frac{1}{2}\right)(\tan\beta - \beta) - \frac{\pi}{4}\right], \quad (19)$$

where

$$\cos\beta = L/pr \quad (20)$$

remains finite in the semiclassical limit  $\hbar \rightarrow 0$ . The asymptotic formula (19) is valid for  $r > L/p$ . In the "forbidden" region  $r < L/p$ , a different asymptotic equation must be used. It can be shown without difficulties, that the forbidden regions  $r < L/p$  and  $r < r_0$  give vanishing contributions to the integral (4) for the  $T$ -matrix elements in the semiclassical limit. Inserting Eqs. (18) and (19) into integral (4), and rearranging the terms after rewriting the trigonometric functions as exponentials, we obtain for the half-shell  $T$ -matrix elements

$$t_i(p, p_E; E) = \frac{1}{2\pi\hbar} \frac{1}{p(p_E)^{1/2}} e^{i\eta_l} \times [I_{+}^{*} + I_{-}^{*} - i(I_{+}^{*} - I_{-}^{*})], \quad (21)$$

with

$$I_{\pm}^{*} = \int_{\max(r_0, L/p)}^{\infty} \frac{drV(r)}{[p_i(r)\sin\beta]^{1/2}} e^{\pm(i/\hbar)H_{\pm}(r)}, \quad (22)$$

where

$$H_{\pm}(r) = \int_{r_0}^r p_i(r') dr' \pm \left( [(pr)^2 - L^2]^{1/2} - L \cos^{-1} \frac{L}{pr} \right). \quad (23)$$

The upper  $\pm$  index of  $I_{\pm}^{*}$  refers to  $e^{\pm i}$  and the lower  $\pm$  index to  $H_{\pm}$ . Integrals (22) are evaluated in the limit of small  $\hbar$  using the method of stationary phase (or equivalently the method of steepest descent if the stationary points are complex):

$$\int_{\gamma} dz g(z) \exp\left(\frac{i}{\hbar} f(z)\right) dz \approx \left( \frac{2\pi\hbar}{|f''(z_s)|} \right)^{1/2} g(z_s) \times \exp\left[\frac{i}{\hbar} f(z_s) + \frac{i}{2} \left( \frac{\pi}{2} - \arg f''(z_s) \right)\right]. \quad (24)$$

The point  $z_s$  ("saddle point" or "stationary point") is determined by  $f'(z_s) = 0$ .  $z_s$  must be a point on the integration path  $\gamma$  and the real part of  $(i/\hbar)f(z)$  must have a strict maximum at  $z_s$  along  $\gamma$ . If these conditions are not met (for instance if  $z_s$  is not a point on  $\gamma$ ), then the integration path must be transformed according to Cauchy's deformation theorem. The evaluation of integrals by this method is one of the central points of the semiclassical approximation scheme.<sup>12-14</sup> Looking for the stationary points  $r_s$  we find

$$\frac{d}{dr} H_{\pm}(r) \Big|_{r_s} = p_i(r_s) \pm p \left[ 1 - \left( \frac{L}{pr_s} \right)^2 \right]^{1/2} = 0. \quad (25)$$

There is no solution of this equation in the  $H_{+}$  case, and so the integrals  $I_{+}^{*}$  give no contribution in the semiclassical limit. For  $I_{-}^{*}$ , Eq. (25) can be conveniently written

$$p_E^2 - p^2 = 2mV(r_s); \quad (26)$$

i.e., at the stationary point  $r_s$  the kinetic energy is equal to  $p^2/2m$ . In the following discussion we will assume for simplicity, that the potential  $V(r)$  is purely repulsive, i.e., monotonically decreasing. In this case Eq. (26) defines three regions:

- (I)  $p < p_{\min}$ , classically forbidden ( $r_s < r_0$ );
- (II)  $p_{\min} < p < p_E$ , classically allowed ( $r_0 < r_s$ );
- (III)  $p_E < p$ , classically forbidden ( $r_s$  complex);

where

$$p_{\min} = L/r_0 \quad (27)$$

is the momentum at the classical turning point. "Classically allowed" means that a classical particle with angular momentum  $L$  and energy  $E$  will reach the momentum  $p$  somewhere on its trajectory, and "classically forbidden" means that the momentum  $p$  is not possible. Nevertheless, this may be the case for complex trajectories, i.e., complex-valued solutions of the classical equations of motion.<sup>14</sup> In the classically allowed region II both integrals  $I_{\pm}^{\dagger}$  contribute, in the forbidden region I the stationary point  $r_s$  is on the wrong sheet for the integral  $I_{-}^{\dagger}$ , and so only  $I_{+}^{\dagger}$  contributes in this region. In region III we have pairs of complex-conjugate saddle points  $r_s$  for each integral  $I_{\pm}^{\dagger}$  and the "correct" one must be chosen carefully.<sup>14</sup> This is indicated by an exponentially damped contribution, which vanishes for  $\hbar \rightarrow 0$ . With

$$\left. \frac{d^2}{dr^2} H_{-}(r) \right|_{r_s} = - \frac{mV'(r_s)}{p_I(r_s)}, \quad (28)$$

we obtain the final result for the half-shell matrix elements, which is conveniently written

$$t_I(p, p_E; E) = e^{i\eta_I} \text{Im} \chi_I(p, p_E), \quad (29)$$

where  $\text{Im} \chi_I$  is the imaginary part of

$$\chi_I(p, p_E) = \frac{p^2 - p_E^2}{m[2\pi m \hbar p p_E |p_I(r_s) V'(r_s)|]^{1/2}} \times \begin{cases} \frac{1}{2} \exp[i(\eta_I(p) - \frac{1}{2}\pi)], & p < p_{\min}; \\ \exp\{i(\eta_I(p) - \frac{1}{4}\pi)\}, & p_{\min} < p < p_E; \\ \exp\{i[\eta_I(p) - \frac{1}{2} \arg(-p_I(r_s) V'(r_s)) - \frac{1}{4}\pi]\}, & p_E < p. \end{cases} \quad (30)$$

The off-shell scattering phase shift  $\eta_I(p) = \hbar H_{-}(r_s)$  is given by

$$\eta_I(p) = \frac{1}{\hbar} \left( \int_{r_0}^{r_s} p_I(r') dr' - [(p r_s)^2 - L^2]^{1/2} + L \cos^{-1} \frac{L}{p r_s} \right). \quad (31)$$

$\eta_I(p)$  is purely imaginary for  $p < p_{\min}$ , real in the

classically allowed region  $p_{\min} < p < p_E$ , and complex for  $p_E < p$ . On the energy shell it is identical with the WKB scattering phase shift in Eq. (14):

$$\eta_I(p_E) = \eta_I. \quad (32)$$

The half-shell matrix elements given in Eqs. (29)–(31) obviously satisfy Eq. (12) for the exact  $t_I(p, p_E; E)$  and we identify

$$\phi_I(p, p_E) = \text{Im} \chi_I(p, p_E). \quad (33)$$

Before presenting a few results of numerical calculations we note the following drawbacks of the semiclassical approximation:

(i) At the boundary between the classically forbidden region  $p < p_{\min}$  and the classically allowed region  $p > p_{\min}$ , the semiclassical formula diverges because of  $p_I(r_s) = p_I(r_0) = 0$ . Such a behavior is well known for the usual WKB wave function.

(ii) At the second boundary between the allowed region  $p < p_E$  and the forbidden region  $p > p_E$ , the numerator in Eq. (29) vanishes, but so does the denominator, because of the vanishing  $V'(r_s)$  (the stationary point  $r_s$  goes to infinity in the on-shell limit). If the potential falls off quicker than the Coulomb potential at infinity the semiclassical  $t_I(p, p_E, E)$  vanishes in the on-shell limit, whereas in the Coulomb case it remains finite.

(iii) As a consequence of (ii) the on-shell limit of the semiclassical half-shell  $T$ -matrix elements differs from the semiclassical expression for the on-shell matrix elements.

To provide some quantitative insight into the quality of the semiclassical approximation we present some numerical results for potentials of the inverse-power type.<sup>21</sup> For  $V(r) = ar^{-2}$  ( $a > 0$ ) the exact half-shell matrix elements can be calculated in closed form (see the Appendix) and also the off-shell scattering phase shifts (30) can be evaluated analytically. It turns out that  $m p_E t_I(p, p_E; E)$  does only depend on  $p/p_E$ , the angular quantum number  $l$  and the parameter  $\Lambda = (2ma/\hbar)^{1/2}$ , which is a measure of the classicality of the problem. For the  $r^{-2}$  potential the WKB phase shift  $\eta_I$  is exact<sup>22</sup> and therefore it is only necessary to compare the quantities  $m p_E e^{-i\eta_I} t_I(p, p_E; E)$ , which are real, according to Eq. (12).

Figures 1–4 show typical results for  $l=0$ ,  $l=2$ , and two values of the classicality parameter  $\Lambda = 2$  and  $\Lambda = 7$ . Away from the pole at  $p_{\min}$  and the zero at  $p_E$  the semiclassical approximation is in good agreement with the exact values, especially for larger values of  $\Lambda$ . The agreement is surprisingly good in view of the low values of the angular-momentum quantum numbers. The figures show the following characteristics of the  $T$ -matrix elements: We have a classically allowed region, where the matrix elements are oscillatory and

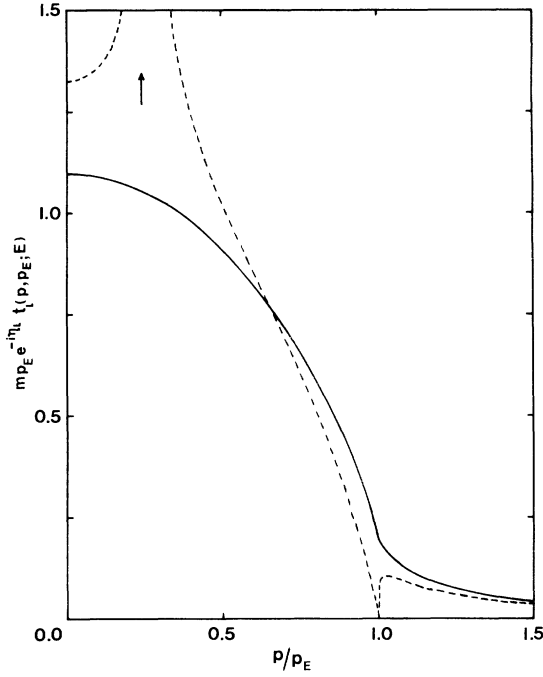


FIG. 1. Half-shell  $T$ -matrix elements  $m p_E e^{-i\eta_l} t_l(p, p_E; E)$  for the  $a/r^2$  potential as function of  $p/p_E$ ;  $\Lambda = (2ma)^{1/2}/\hbar = 2$  and angular-momentum quantum number  $l=0$ . The exact result (full curve) is compared with the semiclassical result (broken curve). The semiclassical approximation diverges for  $p=p_{\min}$  and is zero for  $p=p_E$ . The position of  $p_{\min}$  is marked by an arrow.

large. This region is surrounded by classically forbidden regions, where the matrix elements are exponentially damped. The magnitude of the  $t_l$  is largest for  $p \gtrsim p_{\min}$ , as already observed by Brumer and Shapiro.<sup>7,8</sup>

#### B. Off-shell wave function and off-shell matrix elements

In order to obtain a semiclassical approximation to the off-shell  $T$ -matrix elements we first derive a WKB-type approximation to the off-shell wave function, i.e., to the solution of the inhomogeneous differential equation (5). Inserting the ansatz  $A(r)\hat{j}_l(p r/\hbar)$ —which is motivated by the exact solution for  $V(r)=\text{const.}$ —into Eq. (5) and expanding  $A(r)$  in powers of  $\hbar$  we obtain in lowest order of  $\hbar$  a special solution of the inhomogeneous differential equation (5) with

$$A(r) = \frac{p_E^2 - p^2}{p_E^2 - p^2 - 2mV(r)}. \quad (34)$$

This approximation is invalid in the neighborhood of  $r_s$ , where the denominator of Eq. (34) vanishes. The final solution of Eq. (5), which satisfies the boundary condition (8) is obtained by adding the

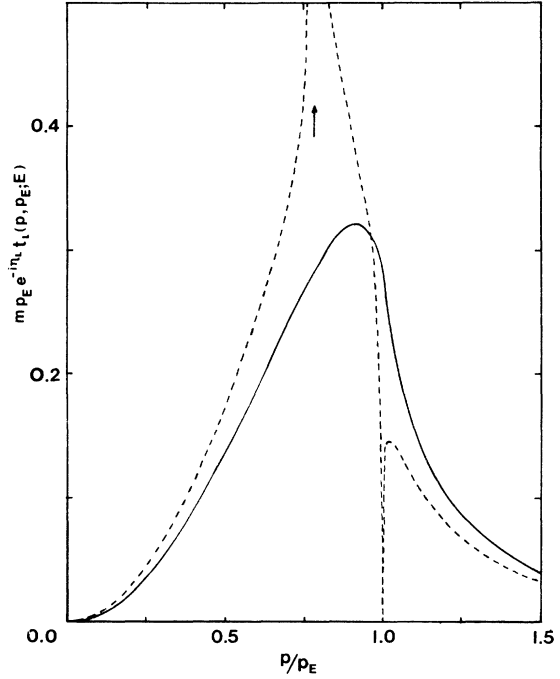


FIG. 2. Same as Fig. 1;  $\Lambda=2$  and  $l=2$ .

proper semiclassical solution (17 a, b) of the homogeneous equation, i.e., for  $r < r_s$  the WKB wave function  $\psi_i^{(1)}(r)$ , which is exponentially decreasing for small  $r$ , and for  $r > r_s$  the asymptotically outgoing wave function  $\psi_i^{(2)}$ :

$$\begin{aligned} \omega_i(r, p; E) &= \frac{p_E^2 - p^2}{p_E^2 - p^2 - 2mV(r)} \hat{j}_l(p r/\hbar) \\ &\quad - \pi m p t_l(p, p_E; E) e^{-i\eta_l} \psi_i^{(2)}(r) \end{aligned} \quad \text{for } r > r_s. \quad (35)$$

This approximation is invalid in the neighborhood of  $r_s$  and  $r_0$ . The final result for the semiclassical off-shell  $T$ -matrix elements is obtained by inserting the semiclassical expression for the off-shell wave function into integral (4) and evaluating the integral by means of the method of steepest descent. The inhomogeneous term in Eq. (35) gives a vanishing contribution in the semiclassical limit for  $p \neq p'$  and the contribution of the other term can be calculated in the same way as in the half-shell case. The final off-shell approximation is

$$t_l(p, p'; E) = -\pi m p_E \chi_l(p_>, p_E) \text{Im} \chi_l(p_<, p_E), \quad (36)$$

with  $p_> = \max(p, p')$  and  $p_< = \min(p, p')$ .

The half-shell limit of the off-shell approximation is zero (for potentials falling off quicker than  $r^{-1}$  at infinity) and not identical with the half-shell semiclassical approximation (29), just as the on-shell limit of the half-shell expression. Figure 5 illustrates the different regions in the  $(p', p)$  plane.

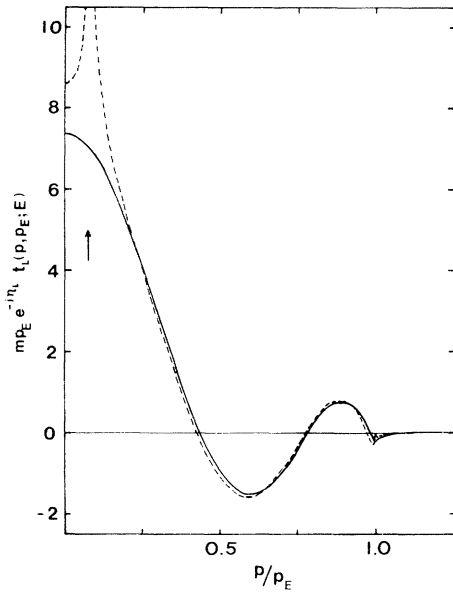


FIG. 3. Same as Fig. 1;  $\Lambda=7$  and  $l=0$ .

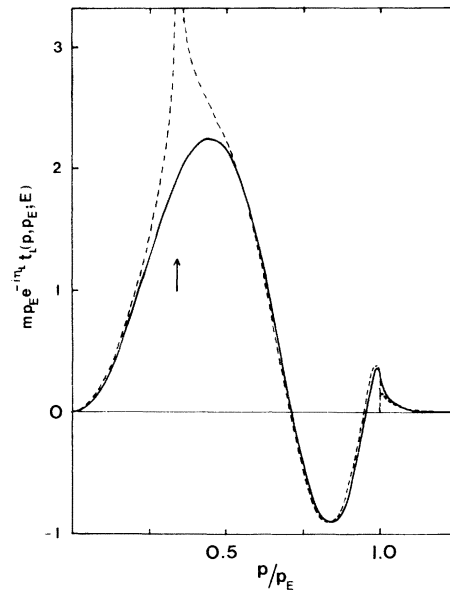


FIG. 4. Same as Fig. 1;  $\Lambda=7$  and  $l=2$ .

Region (A) is classically allowed, i.e., there is a classical trajectory with energy  $E$  and angular momentum  $L$ , which joins the two momenta  $p$  and  $p'$ . The  $t_l(p, p'; E)$  are large and oscillatory in  $p$  and  $p'$ . The regions HF are half-forbidden, the  $t_l(p, p'; E)$  are oscillatory in  $p$  or  $p'$ . The regions CF are classically completely forbidden and the matrix elements are very small. In the classically forbidden regions there is no real classical trajectory on which the momenta  $p$  and  $p'$  occur, but there is a complex-valued classical trajectory, which joins the two momenta.<sup>14</sup> On the line  $p=p'$  the real part of the first derivative is discontinuous, the imaginary part is continuous. This behavior has its origin in the neglect of the inhomogeneous term of Eq. (35), which is only valid for  $p' \neq p$ .

The following properties of the semiclassical approximation (36) should be pointed out:

(a) The off-shell behavior of the  $t_l$  is completely determined by the half-shell expression  $\chi_l(p, p_E)$  [but not by the half-shell matrix elements  $t_l(p, p_E; E)$ , i.e., not by the imaginary part of  $\chi_l(p, p_E)$ ].

(b) The semiclassical approximation (36) is obviously symmetric in  $p$  and  $p'$ .

(c) The off-shell unitarity relation (13) is satisfied because of

$$\begin{aligned} \text{Im} l_l(p, p'; E) &= -\pi m p_E \text{Im} \chi_l(p_>, p_E) \cdot \text{Im} \chi_l(p_<, p_E) \\ &= -\pi m p_E \phi_l(p, p_E) \phi_l(p', p_E). \end{aligned} \tag{37}$$

This is a very important feature of the semiclass-

sical formula for the  $t_l$ .

Numerical sample calculations were performed for inverse power potentials  $V(r) = \epsilon(R/r)^n$ , which are extensively used in atomic scattering at high energies.<sup>23</sup> For these potentials  $m p_E t_l(p, p'; E)$  as a function of  $l$  and the reduced momenta  $p/p_E$ ,  $p'/p_E$  depends only on two dimensionless parameters: the reduced energy  $E_R = E/\epsilon$  and a "classicality" parameter  $K_R = p_E R/\hbar$ . The stationary points  $r_s$  can be calculated analytically. The integral in Eq. (31) for the off-shell scattering phase shift  $\eta_l(p)$  is evaluated by means of the

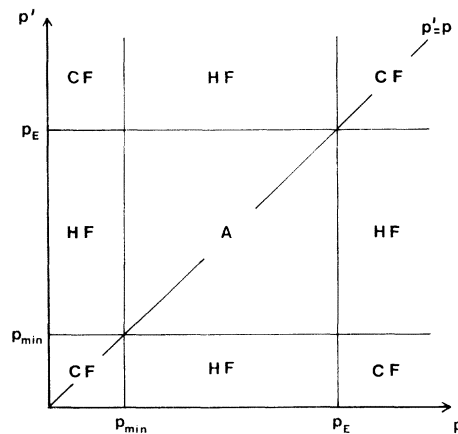


FIG. 5. Sketch of the classically allowed (A), classically half (HF), and completely (CF) forbidden regions in the  $(p, p')$  plane.  $t_l(p, p'; E)$  is large and oscillatory in region (A) and small and exponentially damped in regions (CF). The semiclassical approximation diverges if  $p$  or  $p'$  is equal to  $p_{\min}$ .

usual Gauss-Mehler integration,<sup>24</sup> which works also in the forbidden (complex-valued) case. As a typical example Fig. 6 shows real and imaginary parts of the matrix elements for the  $r^{-12}$  potential ( $p' = 0.8p_E, l = 10$ ) as a function of  $p/p_E$ . Reduced energy and "classicality" are  $E_R = 2$  and  $K_R = 60$ . For the  $r^{-12}$  potential the matrix elements are far more oscillatory than for the  $r^{-2}$  potential. The different phase behavior for  $p < p'$  and  $p > p'$  arises from the change in the real part at  $p = p'$  as discussed above.

#### IV. CONCLUDING REMARKS

A semiclassical approximation to the off-shell  $T$ -matrix elements for local potentials is derived. The approximation satisfies the off-shell unitarity relation and permits a fast calculation of the  $t_l(p, p'; E)$ . We found good agreement with exact results under semiclassical conditions. Moreover, the semiclassical theory gives an insight into the structure of the matrix elements, the regions, where the matrix elements are large, and so on. The semiclassical approximation breaks down at the boundary between classically allowed and forbidden regions. It should be possible, however, to overcome these drawbacks by means of a uniform approximation, similar to the successful uniform approximations in potential scattering.<sup>13</sup>

In the present paper the potential is assumed to be purely repulsive. An extension to attractive potentials and potentials with a minimum is straightforward and will be the topic of future studies.

#### APPENDIX

For the potential  $V(r) = ar^{-2}$  the half-shell  $T$ -matrix elements can be calculated in closed form. In this case the wave function with the correct normalization (8) is given by

$$\omega_l(r, p_E; E) = e^{i\eta_l} \hat{j}_\lambda(p_E r / \hbar), \quad (\text{A1})$$

with

$$\eta_l = \frac{1}{2} \pi (l - \lambda) \quad (\text{A2})$$

and

$$\lambda = -\frac{1}{2} + [(l + \frac{1}{2})^2 + 2ma/\hbar^2]^{1/2}. \quad (\text{A3})$$

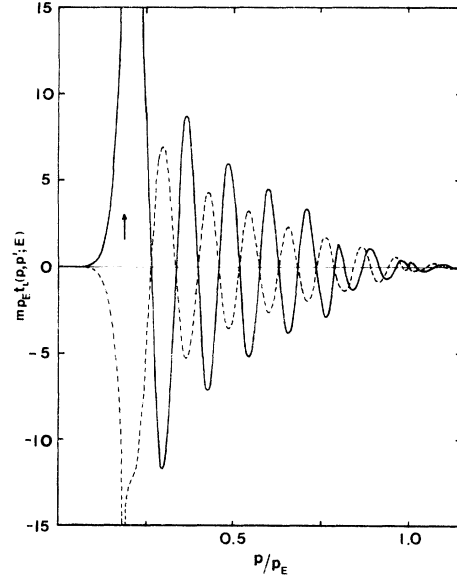


FIG. 6. Off-shell  $T$ -matrix elements  $m p_E t_l(p, p'; E)$  for the  $r^{-12}$  potential as function of  $p/p_E$  for  $p' = 0.8p_E$ . Angular-momentum quantum number  $l = 10$ , reduced energy  $E_R = 2$ , and classicality parameter  $K_R = 60$ . The full curve is the real part and the broken curve is the imaginary part.

This is easily checked by inserting (A1) into the (homogeneous) differential equation (5). Equation (4) for the  $t_l$  reads

$$\begin{aligned} t_l(p, p_E; E) &= \frac{2a}{\pi \hbar p p_E} e^{i\eta_l} \int_0^\infty \hat{j}_l(p r / \hbar) \hat{j}_\lambda(p_E r / \hbar) r^{-2} dr \\ &= \frac{a}{\hbar^2 (p p_E)^{1/2}} e^{i\eta_l} J_{l+1/2, \lambda+1/2}(p r / \hbar, p_E r / \hbar). \end{aligned} \quad (\text{A4})$$

The integral  $J$  is of Weber-Schafheitlin type and can be evaluated in closed form<sup>25</sup>

$$\begin{aligned} J_{\mu, \nu}(k', k) &= \frac{1}{2} \left(\frac{k'}{k}\right)^\mu \frac{\Gamma(\frac{1}{2}(\mu + \nu))}{\Gamma(\mu + 1) \Gamma(\frac{1}{2}(\nu - \mu + 2))} \\ &\quad \times {}_2F_1\left(\frac{1}{2}(\mu + \nu), \frac{1}{2}(\mu - \nu); \mu + 1; (k'/k)^2\right) \end{aligned} \quad (\text{A5})$$

for  $k' < k$ . For  $k' > k$  we make use of the symmetry relation  $J_{\mu, \nu}(k', k) = J_{\nu, \mu}(k, k')$ .  ${}_2F_1$  is the hypergeometric function.

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