Quantum manifestations of bifurcations of closed orbits in the photodetachment cross section of H^- in parallel fields

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(Received 3 June 1996; revised manuscript received 31 January 1997)

In the preceding paper, we showed that the semiclassical approximation diverges at a bifurcation, and that this divergence coincides with the passage of a focused cusp through the origin. Here we obtain a wave function in the vicinity of this cusp, and we use that wave function to eliminate the divergences in the photodetachment cross section. To describe the focused cusp, we first discuss the wave function of an ordinary two-dimensional (nonfocused) cusp. This wave function is known as a Pearcey function, and it has been studied extensively. Then we show how the formulas that lead to the Pearcey function have to be modified to describe a cylindrically focused cusp. The resulting wave function turns out to be given by an integral of Fresnel type containing within it a cylindrical Bessel function. This wave function is used to derive a formula for the photodetachment cross section near a bifurcation. That formula is a simple closed-form expression containing a Fresnel integral. Comparison with exact quantum calculations shows that this corrected-semiclassical formula is quite accurate. [S1050-2947(97)03406-9]

PACS number(s): 32.80.Gc

I. PHYSICAL IDEAS AND NUMERICAL CALCULATIONS

Cusped caustics are familiar objects in ray optics and semiclassical mechanics. A theorem from ‘‘catastrophe theory’’ asserts that such cusps are one of the two generic forms of caustics in a plane [1]. It is well known that at a simple boundary between classically allowed and classically forbidden regions (a fold caustic) the divergent primitive-semiclassical wave function must be replaced by an Airy function, which is smooth at the caustic and which describes diffraction or tunneling into the classically forbidden region. For a cusped caustic, the relevant diffraction integral is known as a Pearcey function. Photographs, contour plots, and formulas for this function are given in Ref. [2].

Our structure [3] is slightly different: the cusp lies on an axis of cylindrical symmetry, so it is not one of the generic structures. Nevertheless, such focused cusps are familiar structures in geometrical optics [4]: they cause the simplest aberration of the focus of a lens, spherical aberration. The relevant diffraction integrals are closely related to Fresnel integrals [5].

In this paper we show that similar Fresnel-Bessel integrals describe the wave function and the recurrence strength at a bifurcation of the parallel orbit. The derivation we give is of some mild interest in itself—instead of the language of nineteenth-century optics, we use the language of twentieth-century semiclassical mechanics, and particularly the description of trajectories and wave functions in terms of Lagrangian manifolds. This approach is the modern expression of older methods, and it is also more complete and systematic (less ‘‘*ad hoc*’’) than earlier approaches. In the present case, simple trigonometric expressions can be given for all properties of the classical orbits, and therefore this system provides an excellent paradigm for the application of Lagrangian-manifold methods. Indeed, this is the first nontrivial case we have come across in which the whole Lagrangian-manifold formulation of semiclassical theory can be carried out analytically, so it is worthwhile to present it in detail. Finally, the systematic treatment given here provided the foundation for our analysis of a more difficult case, excitation of a neutral atom in an electric field [6].

We show that the wave function near the focused cusp is given by Eq. (5.19). The contribution to the photodetachment cross section near a bifurcation arising from the combined effects of the parallel orbit and the bifurcating orbit is given by Eq. (5.25), with the function F_1 given by Eq. (4.15g).

We have used these formulas to compute corrected-semiclassical photodetachment cross sections. In Fig. 1 we show an energy range close to the fourth bifurcation of the parallel orbit. The heavy line is an ‘‘exact’’ numerical quantum calculation, and the light line is the corrected-semiclassical result. The divergence in the primitive-semiclassical formula has been corrected, and the two formulas agree rather well with each other.

II. CENTRAL PRINCIPLE OF THE DERIVATION

A wave function $\Psi(q_1,\ldots,q_n)$ must be finite everywhere in order to be an acceptable solution to the Schrödinger equation. However, semiclassical approximations to $\Psi(\mathbf{q})$ contain divergences at any boundary between classically allowed and classically forbidden regions, and at any focal point or focal line. ‘‘In general’’ such divergences can be repaired locally by transforming the wave equation to some mixed position-momentum representation, defined as a Fourier transform of the wave function over some selected set of q variables,

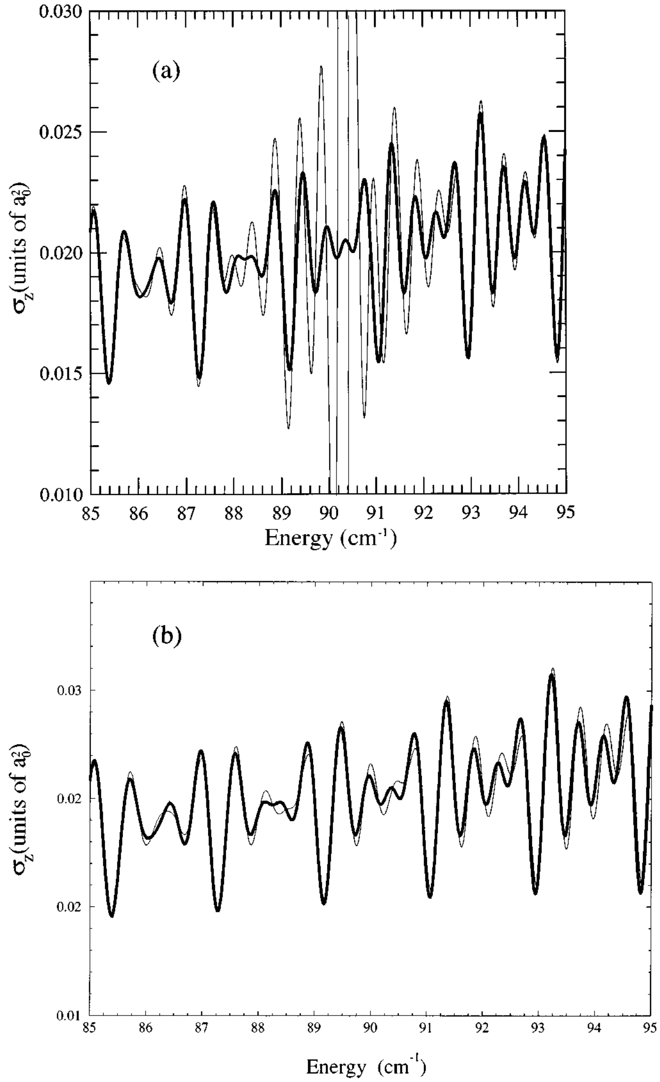

FIG. 1. Exact quantum (heavy line) and semiclassical (light line) calculations of the photodetachment cross section in the vicinity of the fourth bifurcation of the parallel orbit. The cross section is in units of bohrs [2], and the energy in units of cm^{-1}. (a) The primitive-semiclassical approximation has diverging oscillations. (b) The corrected approximation using a Fresnel diffraction integral is much better.

$$\tilde{\Psi}(p_1,p_2,\ldots,p_j,q_{j+1},\ldots,q_n) \equiv (2\pi i\hbar)^{-j/2}\int dq_1\cdots dq_j \times \exp\left[-i\sum_{k=1}^{j} p_k q_k/\hbar\right]\Psi(q_1,\ldots,q_n). \tag{2.1}$$

The integral may be performed over any subset of $(q_1,\ldots,q_n)$ or over all of them [7].

''Almost always,'' there exists a representation in which the semiclassical approximation does not diverge, and, ''for small $\hbar$,'' constitutes an adequate description of the exact wave function in that representation. From that wave function [call it $\tilde{\Psi}(\mathbf{p}_\alpha \mathbf{q}_\beta)$], an accurate configuration-space wave function can be constructed by inverse Fourier transformation,

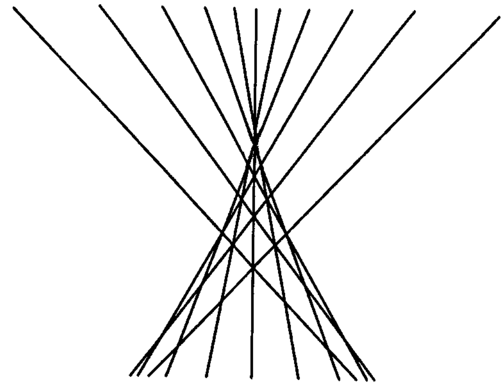

FIG. 2. Classical orbits forming a cusp.

$$\Psi(\mathbf{q}) = (-2\pi i\hbar)^{-j/2}\int \exp[i\mathbf{p}_\alpha\cdot\mathbf{q}_\alpha/\hbar]\tilde{\Psi}(\mathbf{p}_\alpha,\mathbf{q}_\beta)d\mathbf{p}_\alpha. \tag{2.2}$$

This principle has been fully elaborated by Maslov and Fedoriuk [8] and Delos [9].

The words ''in general'' and ''almost always'' have a precise meaning (same as ''generically''). They mean that exceptions to the rule exist, but they are indeed exceptional in the sense of being a set of measure zero in some suitably defined space. In physics, we find exceptional cases regularly because we often deal with systems having special symmetries. In the present case, our system has cylindrical symmetry, so it is quite nongeneric, and we must consider the possibility that the general principle might fail. In fact, we find that it works. A good description of the wave function for the focused cusp $\tilde{\Psi}(x,y,z)$ is obtained by transforming x and y to p_x and p_y, constructing a semiclassical approximation in the mixed space $\tilde{\Psi}(p_x,p_y,z)$, and then transforming back using Eq. (2.2).

III. THE WAVE FUNCTION FOR A TWO-DIMENSIONAL CUSP

As stated earlier, formulas for the focused cusp can be derived as natural modifications of the formulas for an ordinary two-dimensional cusp. Here we set up those formulas in a manner that will lead us to the necessary modifications.

A. Classical orbits locally forming a cusp

As always, semiclassical wave functions are constructed from properties of orbits of classical particles, so we begin by forgetting quantum mechanics, and discuss only classical orbits.

1. A free-particle cusp

We define a ''free-particle cusp'' as an arrangement of classical orbits having the following properties. (1) In the relevant domain of configuration variables $\mathbf{q}=(x,z)$, the particle moves under the Hamiltonian

$$H(p_x,p_z,x,z) = (p_x^2+p_z^2)/2m, \tag{3.1}$$

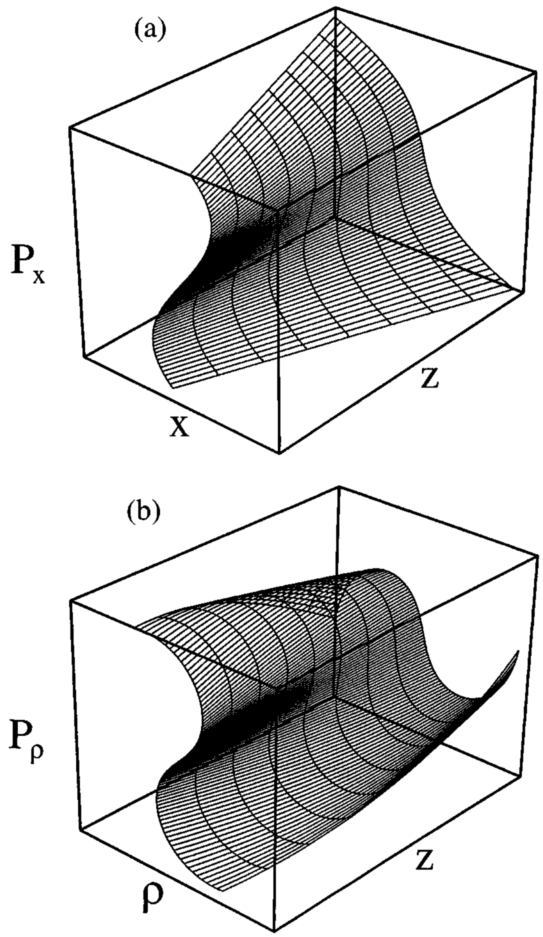

FIG. 3. Lagrangian manifolds associated with cusps. (a) For a free-particle cusp, the manifold is a surface that can be ruled by straight lines organized so that sections form sigmoid curves. (b) Equations (5.1) give curved orbits that form a more complex global structure, but a similar local structure.

i.e., $\dot{x}=p_x/m$, $\dot{z}=p_z/m$, $\dot{p}_x=\dot{p}_z=0$, so all orbits are straight lines. (2) All orbits have the same value of H, so the motion on all is at the same fixed speed. (3) The orbits come together in the geometrical structure shown in Fig. 2. This structure will be defined further by formulas given below.

2. The Lagrangian manifold and its canonical generator

The orbit structure shown in Fig. 2 can also be described by a smooth two-dimensional ruled surface in the four-dimensional $(p_x p_z x z)$ phase space (Fig. 3). That surface is called a Lagrangian manifold. It has the following properties. (1) The variables p_x and z can be used as coordinates spanning the relevant local domain of the manifold. (2) There exists a canonical generator $\tilde{S}(p_x,z)$ such that the embedding of the manifold in phase space is described by the two functions [10]

$$x(p_x,z)=-\partial\tilde{S}(p_x,z)/\partial p_x, \tag{3.2a}$$

$$p_z(p_x,z)=\partial\tilde{S}(p_x,z)/\partial z. \tag{3.2b}$$

(3) The generator satisfies the Hamilton-Jacobi equation in (p_x,z) space,

$$\frac{1}{2m}\left[p_x^2+\left(\frac{\partial\tilde{S}(p_x,z)}{\partial z}\right)^2\right]-E=0. \tag{3.3}$$

(4) The relevant generator for our cusp is

$$\tilde{S}(p_x,z)=S_c-(2mE-p_x^2)^{1/2}(z-z_c)+\tilde{S}_2(p_x), \tag{3.4a}$$

$$\tilde{S}_2(p_x)=\tfrac{1}{4}\alpha p_x^4+\cdots\ . \tag{3.4b}$$

Equation (3.4a) satisfies Eq. (3.3) for any $\tilde{S}_2(p_x)$; later we will show that the cusp structure is obtained if the power series expansion of $\tilde{S}_2(p_x)$ starts at the quartic term. The parameter z_c will become the tip of the cusp, and for p_z negative, the cusp points upward if α is positive. $\tilde{S}_c$ is an arbitrary additive constant. The whole generating function will later become the phase of the wave function $\tilde{\Psi}(p_x,z)$.

From Eqs. (3.2) and (3.4), the surface shown in Fig. 3 is specified by the formulas

$$p_z(p_x,z)=p_z(p_x)=-(2mE-p_x^2)^{1/2}\equiv-(P^2-p_x^2)^{1/2}, \tag{3.5a}$$

$$x(p_x,z)=p_x(z-z_c)/p_z(p_x)-\alpha p_x^3+\cdots\ , \tag{3.5b}$$

which is called the canonical representation of the Lagrangian manifold. For future reference, we note that

$$\frac{\partial x(p_x,z)}{\partial p_x}=P^2(z-z_c)/p_z^3(p_x)-3\alpha p_x^2+\cdots\ , \tag{3.5c}$$

where

$$P=(p_x^2+p_z^2)^{1/2}=(2mE)^{1/2}>0. \tag{3.5d}$$

3. Local parametric representation of the cusp manifold

The same two-dimensional surface and its generator can also be represented parametrically, by using two alternative variables (t',θ') to span the manifold, and specifying $\mathbf{q}(t',\theta')$, $\mathbf{p}(t',\theta')$, and $\tilde{S}(t',\theta')$. Each orbit is labeled by its angle θ', and the position along each orbit is defined by the local time variable t':

$$p_z(t',\theta')=-P\cos\theta',$$

$$p_x(t',\theta')=-P\sin\theta',$$

$$z(t',\theta')=-Pt'/m\cos\theta'+z_0(\theta'),$$

$$x(t',\theta')=-Pt'\sin\theta'/m. \tag{3.6}$$

The cusp structure is contained in the function $z_0(\theta')$, which is the location on the z axis at which the orbit having angle θ' crosses $x=0$. This quantity can be related to the parameters (z_c,α) in the canonical representation by setting $x=0$ in Eq. (3.5b) and solving for z, which then represents $z_0(\theta')$:

$$z(x=0)=z_0(\theta')=z_c-\alpha p_x^2 p_z(p_x)+\cdots \tag{3.7a}$$

$$=z_c-\alpha P^3\sin^2\theta'\cos\theta'+\cdots \tag{3.7b}$$

and

$$z(t',\theta')=z_c-\alpha P^3\sin^2\theta'\cos\theta'-(Pt'/m)\cos\theta'+\cdots \tag{3.7c}$$

$$\simeq z_c-\alpha P^3\theta'^2-(Pt'/m)\cos\theta'+\cdots . \tag{3.7d}$$

A local parametric representation of the canonical generator follows immediately,

$$\tilde{S}(t',\theta')=\tilde{S}(p_x(t',\theta'),z(t',\theta'))$$
$$=P^2t'\cos^2\theta'/m+\alpha P^4(\sin^2\theta'-\tfrac{3}{4}\sin^4\theta')+\cdots . \tag{3.8}$$

The ''configuration-space generator'' is defined such that

$$S(\mathbf{q})\equiv S(x,z)\equiv\tilde{S}(p_x(x,z),z)+p_x(x,z)x. \tag{3.9a}$$

This quantity does not have a good representation inside the cusp, because three sheets of the manifold project to a single point in configuration space. However, it does have a good parametric representation,

$$S(t',\theta')=P^2t'/m+\alpha P^4(\sin^2\theta'-\tfrac{3}{4}\sin^4\theta') \tag{3.9b}$$

$$\simeq P^2t'/m+\alpha P^4\theta'^2+\cdots . \tag{3.9c}$$

[This quantity is related to the phase of the configuration-space wave function $\Psi(x,z)$.]

4. Jacobians and the local structure of the cusp

The density of particles flowing along classical orbits is related to Jacobians defined either in (x,z) space, (p_x,z) space, or in the parametric representation (t',θ').

First let us define

$$\tilde{J}(p_x,z)\equiv\tilde{J}(t',\theta')\equiv\frac{\partial(p_x,z)}{\partial(t',\theta')}=-P^2\cos^2\theta'/m=-p_z^2/m=-(P^2-p_x^2)/m. \tag{3.10}$$

The derivatives follow from Eq. (3.6). This Jacobian is inversely proportional to the particle density as seen in (p_x,z) space. Since p_z is nonzero in the vicinity of the cusp, this density is finite.

The corresponding configuration-space density is inversely proportional to the Jacobian

$$J(x,z)\equiv J(t',\theta')\equiv\frac{\partial(x,z)}{\partial(t',\theta')}=\left(\frac{\partial x}{\partial p_x}\right)\tilde{J}. \tag{3.11}$$

This quantity vanishes only when $(\partial x/\partial p_x)$ vanishes. To find these points (i.e., to find the caustic) we first ''solve'' $\partial x/\partial p_x=0$ for p_x,

$$3\alpha p_x^2=P^2(z-z_c)/p_z^3(p_x)+\cdots ,$$

on the right-hand side approximate $p_z\simeq-P$ if p_x is small, and then substitute the result into (3.5b) to show that the caustic occurs when

$$x(z)=\pm2[(z_c-z)/3\alpha P]^{3/2}+\cdots . \tag{3.12}$$

This is the characteristic formula for a cusped caustic, $x(z)\propto(z_c-z)^{3/2}$; as stated earlier, z_c is the tip of the cusp, and the cusp opens downward for $\alpha>0$ if $p_z<0$.

Additional information is obtained from the parametric representation of the configuration-space Jacobian. From Eqs. (3.6),

$$J(t',\theta')=\frac{\partial(x,z)}{\partial(t',\theta')}$$
$$=-\frac{P^2}{m^2}t'+\frac{\alpha P^4}{m}(2\sin^2\theta'-3\sin^4\theta'). \tag{3.13}$$

(i) If $\theta'=0$, then $J(t',0)$ passes through zero from positive to negative at $t'=0$. This point ($\theta'=0$, $t'=0$) is located at ($x=0$, $z=z_c$), i.e., at the tip of the cusp.

(ii) For $\theta'=0$, we need to evaluate J ($x=0$, $z=0$). This quantity is inversely proportional to the classical density of particles moving parallel to the z axis through the origin. From Eqs. (3.7d) and (3.13) evaluated at $\theta'=0$,

$$J(x=0,\ z=0)=-Pz_c/m\equiv J_\parallel . \tag{3.14}$$

We see that if $z_c<0$ (cusp is below the origin), $J_\parallel$ is negative; when the cusp touches the origin ($z_c=0$), $J_\parallel$ vanishes, and the classical density goes to infinity; finally when the cusp is above the origin, $J_\parallel$ is positive.

(iii) In the last case, $z_c>0$, there is another orbit passing through the origin at some angle. We need the Jacobian associated with that ''new'' orbit, J_ν. From Eq. (3.7d) we find that this orbit approaches at an angle.

$$\theta'^2=z_c/\alpha P^3,$$

so again using Eq. (3.13),

$$J_\nu=2Pz_c=-2J_\parallel . \tag{3.15}$$

The Jacobian associated with the new orbit at the origin is minus twice that associated with the parallel orbit. When the cusp is above the origin, the Jacobian for the parallel orbit has undergone one more sign change than has that for the new orbit.

This fact has consequences for the Maslov indices. It means that for a two-dimensional cusp, the Maslov index μ for the parallel orbit will be equal to that of the new orbit plus one. As the cusp passes through the origin, the Maslov index of the parallel orbit increases by 1, and the Maslov index of the newly created orbit is equal to that of the parallel orbit just before the bifurcation [11].

B. The local wave function for a two-dimensional cusp

We now obtain a local semiclassical approximation for a wave function near the cusp. A primitive-semiclassical wave function is constructed following the standard rules. We start by specifying some initial line or curve in (x,z) space, the points of which are denoted x_0,z_0. At each initial point we need to have the wave function $\Psi(x_0,z_0)$ given. We follow trajectories from each initial point (x_0,z_0) to each point (x,z). Then

$$\Psi(x,z)=\Psi(x_0,z_0)|J(x_0,z_0)/J(x,z)|^{1/2} \times \exp i[S(x,z)/\hbar-\mu\pi/2], \tag{3.16}$$

where J and S are, respectively, the Jacobian and the classical action integrated from (x_0,z_0) to (x,z), and μ is the Maslov index. The points (x_0,z_0) are regarded as functions of (x,z). Inside the cusp, three trajectories pass through every point, so the wave function is a sum of three such terms. As shown earlier, $J(x,z)$ vanishes on the cusped caustic, so this wave function diverges on those curves.

A suitable mixed representation gives a valid semiclassical approximation. Since the Lagrangian manifold has (locally) a good projection into (p_x,z) space, we can use that representation instead. Again starting from some initial curve $\{p_{x_0},z_0\}$, on which $\Psi(p_{x_0},z_0)$ is known, we again follow trajectories to final points (p_x,z), and

$$\tilde{\Psi}(p_x,z)=\Psi(p_{x_0},z_0)|\tilde{J}(p_{x_0},z_0)/\tilde{J}(p_x,z)|^{1/2} \times \exp i[\tilde{S}(p_x,z)/\hbar-\nu\pi/2], \tag{3.17}$$

where ν is the Maslov index for the mixed representation. In the present case, we take $\tilde{S}(p_x,z)$ from Eq. (3.4) and $\tilde{J}(p_x,z)$ from Eq. (3.10), to obtain

$$\tilde{\Psi}(p_x,z)=\Psi(p_{x_0},z_0)|\tilde{J}(p_{x_0},z_0)|^{1/2}|m/p_z^2(p_x)|^{1/2} \times \exp\{i[p_z(p_x)(z-z_c)+\tfrac{1}{4}\alpha p_x^4]/\hbar-i\nu\pi/2\}. \tag{3.18}$$

As stated earlier, in the vicinity of the cusp, p_z does not vanish, so this representation is credible. The corresponding configuration-space wave function is

$$\Psi(x,z)=(-2\pi i\hbar)^{1/2}\int_{-\infty}^{\infty}\exp(ip_x x/\hbar)\tilde{\Psi}(p_x,z)dp_x. \tag{3.19}$$

Near the cusp, it can be reduced to a Pearcey function. Connor [2b] defines the Pearcey function as

$$U(\xi,\eta)=\int_{-\infty}^{\infty}\exp[i(\tfrac{1}{4}u^4-\xi u^2-\eta u)]du. \tag{3.20}$$

If we substitute Eq. (3.18) into Eq. (3.19), expand p_z in powers of $p_x(p_z\simeq -P+p_x^2/2P)$, and approximate everything except the exponential by constants, we find

$$\Psi(x,z)=\frac{\text{const}}{\hbar^{1/2}}\exp[-iP(z-z_c)/\hbar-i\nu\pi/2] \times\int_{-\infty}^{\infty}\exp\left\{i\left[\frac{1}{4}\alpha p_x^4+\frac{z-z_c}{2P}p_x^2+xp_x\right]\Big/\hbar\right\}dp_x \tag{3.21a}$$

$$=\text{const}\times\exp[-iP(z-z_c)/\hbar-i\nu\pi/2]\cdot(\alpha/\hbar)^{1/4} \times U((z_c-z)/2P(\hbar\alpha)^{1/2},x/\hbar^{3/4}\alpha^{1/4}). \tag{3.21b}$$

Plots and pictures of these diffraction functions near a cusp are given in Ref. [2].

[At a lower level of accuracy, one can evaluate the integral (3.21a) by the stationary-phase method. That gives back the primitive-semiclassical approximation, with all its divergences intact. At a higher level of accuracy, one can expand the preexponential factor in powers of p_x and $(z-z_c)$. The resulting refined version of Eq. (3.21b) would also contain derivatives of $U(\xi,\eta)$. Even more refined approximations can be made, by careful mapping of $\tilde{S}(p_x,z)$ onto the standard form $\frac{1}{4}u^4-\xi u^2-\eta u$. We do not need any of those refinements.]

IV. THE WAVE FUNCTION FOR A CYLINDRICAL CUSP

Now we modify the above formulas to construct a wave function for a cylindrically focused cusp. We might be tempted to simply replace p_x by p_ρ, but that will not give the correct result. The cylindrically focused cusp is a three-dimensional object—i.e., the caustic is a two-dimensional surface of revolution in the three-dimensional (xyz) space. The family of orbits is obtained by sweeping Fig. 2 around the z axis. The associated wave functions are focused onto the z axis, and therefore are much more intense on that axis than is predicted by the Pearcey function.

A. Local parametric and canonical representations

As in Eq. (3.1), the local Hamiltonian is now

$$H=(p_x^2+p_y^2+p_z^2)/2m=P^2/2m=E, \tag{4.1a}$$

$$p^2\equiv p_x^2+p_y^2=2mE-p_z^2, \tag{4.1b}$$

$$p_z(p)=-(P^2-p^2)^{1/2}, \tag{4.1c}$$

and the local parametric representation of the orbits is [cf. Eq. (3.6)]

$$p_x(t',\theta',\varphi')=-P\sin\theta'\cos\varphi',$$
$$p_y(t',\theta',\varphi')=-P\sin\theta'\sin\varphi',$$
$$p_z(t',\theta',\varphi')=-P\cos\theta',$$
$$x(t',\theta',\varphi')=p_x(\theta',\varphi')t'/m,$$
$$y(t',\theta',\varphi')=p_y(\theta',\varphi')t'/m,$$
$$z(t',\theta',\varphi')=z_c-\alpha P^3\theta'^2+p_z(\theta',\varphi')t'/m+\cdots,$$
$$\rho(t',\theta'\varphi')=|pt'|/m=|P\sin\theta' t'|/m. \tag{4.2}$$

Suitable canonical coordinates for the Lagrangian manifold are (p_x,p_y,z), and the generator $\tilde{S}(p_x,p_y,z)$ is obtained from Eq. (3.4) through replacing p_x^2 by $p_x^2+p_y^2=p^2$:

$$\tilde{S}(p_x,p_y,z)=S_c-[2mE-(p_x^2+p_y^2)]^{1/2}(z-z_c) +\tilde{S}_2[(p_x^2+p_y^2)^{1/2}],$$
$$\tilde{S}_2(p)=\tfrac{1}{4}\alpha p^4+\cdots. \tag{4.3a}$$

To show that this gives a cylindrically symmetric cusp, we just note that (i) for $p_y=0$ it gives the same picture as the two-dimensional cusp; (ii) $\widetilde{S}(p_x,p_y,z)$ is independent of angle in the p_x,p_y plane. It follows that we can write it as $\widetilde{S}(p,z)$. Various alternative representations will be useful later:

$$\widetilde{S}(p,z)=\widetilde{S}_c-P(z-z_c)+\frac{z-z_c}{2P}\,p^2+\frac{1}{4}\,\alpha p^4+\cdots\,, \tag{4.3b}$$

$$\widetilde{S}(p,z)=\widetilde{S}(p,0)+p_z(p)z, \tag{4.3c}$$

$$\widetilde{S}(p,0)=\widetilde{S}_0-\frac{z_c}{2P}\,p^2+\frac{1}{4}\,\alpha p^4+\cdots\,, \tag{4.3d}$$

$$\widetilde{S}_0=\widetilde{S}_c+Pz_c\,. \tag{4.3e}$$

(4.3f)

[In our Taylor expansions, we drop terms proportional to $(z-z_c)p^4$ and all higher-degree terms.]

From the formulas $x=-\partial\widetilde{S}/\partial p_x$, $y=-\partial\widetilde{S}/\partial p_y$, one can easily show that

$$\rho(p,z)=|\partial\widetilde{S}(p,z)/\partial p|. \tag{4.4}$$

The local Jacobian is equal to p times the Jacobian for the two-dimensional cusp, which we now call $\widetilde{J}_2(p,z)$,

$$\widetilde{J}(p_x,p_y,z)=\left|\frac{\partial(p_x,p_y,z)}{\partial(t',\theta',\varphi')}\right|=p|\widetilde{J}_2(p,z)|=pp_z^2/m, \tag{4.5a}$$

$$=P^3\cos^2\theta'\sin\theta'/m. \tag{4.5b}$$

All the properties of the Jacobian $\widetilde{J}$ that were described in Sec. III A 4 still hold, except that now the two-dimensional Jacobian is multiplied by p. (When the relevant ratio of Jacobians is calculated, that factor will drop out.)

There again exists a configuration-space generator

$$S(\mathbf{q})=\widetilde{S}+p_xx+p_yy=\widetilde{S}+p\rho \tag{4.6}$$

(where p_x and p_y are to be expressed as functions of configuration variables $\mathbf{q}$), and we find that it has the same parametric representation (3.9b), and (3.9c). The configuration-space Jacobian

$$J(x,y,z)=\left|\frac{\partial(x,y,z)}{\partial(t',\theta',\varphi')}\right|=\rho\left|\frac{\partial(\rho,z)}{\partial(t',\theta')}\right|\equiv\rho J_2(\rho,z) \tag{4.7}$$

is equal to ρ times the two-dimensional Jacobian discussed in Eqs. (3.11)–(3.15).

B. Local wave function for the focused cusp

Following the same prescription as before, the wave function is specified on an initial two-dimensional surface in configuration space (such as z_0 equals large positive constant), trajectories are followed to relate (x_0,y_0,z), to (x,y,z), and then

$$\Psi(x,y,z)=\Psi(x_0,y_0,z_0)|J(x_0,y_0,z_0)/J(x,y,z)|^{1/2}\times\exp[iS(x,y,z)/\hbar-\mu\pi/2]. \tag{4.8}$$

Again we combine such terms wherever two or more trajectories contribute. This wave function is well behaved everywhere outside the cylindrical-cusp caustic, but it diverges on that caustic surface [because $J_2(\rho,z)$ vanishes there], and it diverges on the z axis *inside* the cusp (because ρ/ρ_0 vanishes there).

Therefore we go to a mixed representation—appropriate coordinates are (p_x,p_y,z), and this wave function is again calculated by integrating trajectories from an initial surface (p_{x_0},p_{y_0},z_0) on which it is already known:

$$\widetilde{\Psi}(p_x,p_y,z)=\widetilde{A}(p_x,p_y,z)\exp[i\widetilde{S}(p,z)/\hbar-\nu\pi/2], \tag{4.9}$$

$$\widetilde{A}(p_x,p_y,z)=\widetilde{\Psi}(p_{x_0},p_{y_0},z_0)|\widetilde{J}(p_{x_0},p_{y_0},z_0)/\widetilde{J}(p_x,p_y,z)|^{1/2}. \tag{4.10}$$

Then the configuration-space wave function is obtained from the two-dimensional Fourier transform,

$$\Psi(x,y,z)=(-2\pi i\hbar)^{-1}\int\exp[i(p_xx+p_yy)/\hbar]\times\widetilde{\Psi}(p_xp_yz)dp_xdp_y\,. \tag{4.11}$$

At this point, (x,y) and (p_x,p_y) are distinct, independent variables. (On the Lagrangian manifold x and y are functions of p_x and p_y, but here we are integrating over the momentum plane.) Transforming to cylindrical coordinates in both spaces

$$x=\rho\,\cos\varphi,\quad p_x=p\,\cos\varphi_p\,,$$

$$y=\rho\,\sin\varphi,\quad p_y=p\,\sin\varphi_p\,,$$

$$p_xx+p_yy=p\rho\,\cos(\varphi-\varphi_p), \tag{4.12}$$

and presuming that $\widetilde{\Psi}(p_{x_0},p_{y_0},z_0)$ is independent of φ_p, we find that the resulting wave function depends only on ρ and z,

$$\begin{aligned}\Psi(x,y,z)&=\Psi(\rho,z)\\&=\frac{i}{2\pi\hbar}\int\widetilde{A}(p,z)\exp\{i[p\rho\,\cos(\varphi-\varphi_p)\\&\quad+\widetilde{S}(p,z)]/\hbar\}p\;dp\;d\varphi_p\\&=\frac{i}{\hbar}\int\widetilde{A}(p,z)J_0(p\rho/\hbar)\exp[i\widetilde{S}(p,z)/\hbar]p\;dp.\end{aligned} \tag{4.13}$$

Referring back to Eq. (4.3b) we see that we have an integral with at least second and fourth powers of p in the exponent. We need some information about such integrals.

C. Reduction to integrals of Fresnel type

We define integrals of Fresnel type to be those of the form

$$F=\int_0^\infty g(\epsilon)\exp[if(\epsilon)/\hbar]d\epsilon, \tag{4.14}$$

where $g(\epsilon)$, $f(\epsilon)$ are smooth functions of ϵ, $g(0)\neq 0$, $f'(\epsilon)\equiv df(\epsilon)/d\epsilon$ is a monotonically increasing function of ϵ, $g(\epsilon)\to 0$ sufficiently rapidly at large ϵ that there are no questions about convergence. Such an integral has at most one stationary-phase point, $\hat{\epsilon}$, where $f'(\hat{\epsilon})=0$, in the interval $[0,\infty)$. We need suitable approximations for this integral. Those approximations are the following.

(a) If there is a single stationary-phase point $\hat{\epsilon}\geqslant 0$

$$F\to\left(\frac{2\pi\hbar}{|f''(\hat{\epsilon})|}\right)^{1/2} g(\hat{\epsilon})e^{if(\hat{\epsilon})/\hbar}e^{i(\pi/4)\mathrm{sgn}f''(\hat{\epsilon})} + \frac{i\hbar}{f'(0)}\,g(0)e^{if(0)/\hbar}. \tag{4.15a}$$

(b) If there is a stationary-phase point at $\epsilon=0$,

$$F\to\frac{1}{2}\left(\frac{2\pi\hbar}{|f''(0)|}\right)^{1/2} g(0)e^{if(0)/\hbar}e^{i(\pi/4)\mathrm{sgn}f''(0)}. \tag{4.15b}$$

(c) If there is no stationary-phase point near the interval $[0,\infty)$,

$$F\to\frac{i\hbar}{f'(0)}\,g(0)e^{if(0)/\hbar}. \tag{4.15c}$$

(d) Whenever we can truncate Taylor expansions,

$$f(\epsilon)=f_0+\beta\epsilon+\alpha\epsilon^2+\cdots\ , \tag{4.15d}$$

$$g(\epsilon)=g_0+\cdots\ , \tag{4.15e}$$

$$F\to(\hbar/\alpha)^{1/2}F_1(\beta/(\hbar\alpha)^{1/2})g_0e^{if_0/\hbar}, \tag{4.15f}$$

where

$$F_1(\zeta)\equiv\int_0^\infty \exp i(u^2+\zeta u)du \tag{4.15g}$$

is a complex Fresnel integral.

Equation (4.15f) is derived simply by truncating the expansion at the terms listed. The others could then be derived from Eq. (4.15f) by using familiar properties of Fresnel integrals [5]. Actually Eqs. (4.15a)–(4.15c) also hold under somewhat more general conditions—we are looking at stationary-phase integrals with end points [12], and they have been analyzed carefully in Ref. [13].

Now let us reexamine Eq. (4.13). At $\rho=0$, $J_0(p\rho/\hbar)=1$, and [assuming $\widetilde{A}(p,z)\simeq\text{const}$] when we substitute Eq. (4.3b) and change variables to $\epsilon=p^2/2$, we find

$$\Psi(\rho=0,z)=\frac{i}{\hbar}\exp[-iP(z-z_c)/\hbar]\widetilde{A}\times\int_0^\infty \exp(i/\hbar)\left(\alpha\epsilon^2+\frac{z-z_c}{p}\,\epsilon\right)d\epsilon, \tag{4.16a}$$

$$=i(\hbar\alpha)^{-1/2}\exp[-iP(z-z_c)/\hbar]\times F_1((z-z_c)/P(\hbar\alpha)^{1/2})\widetilde{A}. \tag{4.16b}$$

This function is smooth and well behaved for all z, and it contains the contributions from all orbits that pass through $\rho=0$, with all divergences removed. The Bessel function corrects the divergences due to the cylindrical focus, and the Fresnel integral corrects the divergences due to the caustic.

The various asymptotic approximations to this integral given in Eqs. (4.15a)–(4.15c) can be shown to have physical meaning: every term in Eqs. (4.15a)–(4.15c) corresponds to a configuration-space term (4.8). The end point contributions [Eq. (4.15c) or the second term in Eq. (4.15a)] correspond to the ''parallel'' orbit on the z axis that runs straight down through the cusp. The stationary-phase term [first term in Eq. (4.15a)] is present only inside the cusp, and then it corresponds to the new orbit that passes through $\rho=0$ at an angle. The formula (4.15b) applies when the stationary-phase point and the z axis coincide. That is at the tip of the cusp. There the contributions to the full wave function, including the parallel orbit, the new orbit, and their neighbors all coherently focused together, add to one-half of the contribution of the new orbit.

The other important special case occurs when ρ is large enough that $p\rho/\hbar\gg 1$ for relevant values of p. In that case we can use the asymptotic approximation for the Bessel function.

$$J_0(w)=(2\pi w)^{-1/2}(e^{i(w-\pi/4)}+e^{-i(w-\pi/4)}). \tag{4.17}$$

The first of these exponentials gives in Eq. (4.13)

$$\Psi(\rho,z)\sim\left(\frac{2\pi}{\hbar\rho}\right)^{1/2}\exp[-iP(z-z_c)/\hbar]\times\int_0^\infty \exp\left[\frac{i}{\hbar}\left(\frac{\alpha}{4}\,p^4+\frac{z-z_c}{2P}\,p^2+p\rho\right)\right]p^{1/2}dp. \tag{4.18}$$

Comparing with Eq. (2.27a) we see that this wave function is very much like the Pearcey function, but it drops off more rapidly with increasing ρ, as $\rho^{-1/2}$. This is typical of the behavior of any wave function near a cylindrical focus.

The wave function for the focused cusp can be said to be of order unity at large ρ, of order $\hbar^{-1/2}$ everywhere on the z axis, and of order $\hbar^{-1/4}$ on the caustic surface away from the z axis.

V. ''GLOBAL'' WAVE FUNCTION

Everything we did in the previous two sections constituted a local description: the trajectories, manifold, and wave functions were described in a small region of space close to the cusp. Therefore the formulas therein are very general;

they describe orbits and wave functions in the vicinity of any two-dimensional cusp or any three-dimensional cylindrically focused cusp.

Now we need to show that the orbits of an electron in parallel fields actually form such cusps, and we need to evaluate the important parameter α for these cusps. After this is done, we will need to find the wave function in the whole space, the so-called ''global'' (or at least county-wide) wave function. More precisely, we need to connect the local wave function near the cusp with that in other townships; specifically, we have to connect it with the outgoing wave from the atom. This will allow us to evaluate the previously ignored quantities in Eq. (4.10)—the wave function on the initial surface and the ratio of Jacobians. We will find that in the particular case we consider, $\widetilde{A}(p,z)$ is indeed equal to a constant, which we will evaluate [Eq. (5.19)].

A. Returning orbits and cusp structure

In the accompanying paper [3], we gave formulas that here constitute the ''global'' parametric representation of the electron orbits,

$$z(t,\theta_{\rm out})=Pt\,\cos\theta_{\rm out}/m-\tfrac{1}{2}eF_0t^2/m, \tag{5.1a}$$

$$\rho(t,\theta_{\rm out})=(P/m\omega_L)\sin\theta_{\rm out}|\sin\,w_Lt|, \tag{5.1b}$$

$$p_z(t,\theta_{\rm out})=P\,\cos\theta_{\rm out}-eF_0t, \tag{5.1c}$$

$$p_\rho(t,\theta_{\rm out})=P\,\sin\theta_{\rm out}\,\cos(\omega_Lt\,\bmod\pi). \tag{5.1d}$$

[In Eq. (5.1b) we have restricted ρ to be positive. It follows that on one cycle $p_\rho(t,\theta_{\rm out})$ goes from positive to negative, and at the end of the cycle it jumps discontinuously to positive again; that is the meaning of $\cos(\omega_Lt\,\bmod\pi)$ in Eq. (5.1d). Of course this means also that the returning orbits will form only the right-hand half of the cusp.]

In Sec. I it was presumed, as always, that the applied electric and magnetic forces are weak compared to typical atomic forces. As a consequence, anywhere in the vicinity of the origin we can make the approximation that the p's are constant and the q's change linearly with time. Let us define

$$t_N=N\pi/\omega_L=Nt_c, \tag{5.2}$$

which is the time for the Nth return of $\rho(t,\theta_{\rm out})$ to the origin. We assume that at that time $z(t,\theta_{\rm out})$ is also reasonably close to the origin.

From Eq. (5.1)

$$p_z(t_N,\theta_{\rm out})\simeq-p_z(0,\theta_{\rm out})=-P\,\cos\theta_{\rm out},$$

$$p_\rho(t_N,\theta_{\rm out})\simeq-p_\rho(0,\theta_{\rm out})=-P\,\sin\theta_{\rm out}, \tag{5.3}$$

i.e., the direction of motion of the orbit at its return to the origin is exactly opposite to its initial direction. Furthermore, whenever the particle returns close to the origin, there is no angular motion ($p_\varphi=0$) so $p_\rho=\pm(p_x^2+p_y^2)^{1/2}=\pm p$.

We need to expand $\rho(t,\theta_{\rm out})$ and $z(t,\theta_{\rm out})$ in a Taylor series about t_N. The expansion of ρ is trivial:

$$\rho(t,\theta_{\rm out})=P|t-t_N|\sin\theta_{\rm out}/m. \tag{5.4}$$

For the expansion of z, we define z_N as the location of the particle on the parallel orbit at N cyclotron times:

$$z_N\equiv z(t_N,\theta_{\rm out}=0)=Pt_N/m-\tfrac{1}{2}eF_0t_N^2/m. \tag{5.5a}$$

Then, from Eq. (5.1a),

$$z(t,\theta_{\rm out})=z_N+Pt\,\cos\theta_{\rm out}/m-Pt_N/m-\tfrac{1}{2}eF_0(t^2-t_N^2)/m \tag{5.5b}$$

$$\simeq z_N+(Pt_N/m)(\cos\theta_{\rm out}-1)+(P\,\cos\theta_{\rm out}-eFt_N)\times(t-t_N)/m \tag{5.5c}$$

$$\simeq z_N-\frac{Pt_N}{2m}\,\theta_{\rm out}^2+\frac{p_z(t_N,\theta_{\rm out})}{m}\,(t-t_N). \tag{5.5d}$$

Do Eqs. (5.4) and (5.5d) describe a cusp? We compare with Eq. (4.2), the local parametric representation, and we see that they directly correspond. θ' in the local representation is the same as $\theta_{\rm out}$ in the global representation, and t' in the local representation is equivalent to $t-t_N$ in the global representation. The tip of the cusp z_c is at z_N, the position of the particle moving on the parallel orbit at N cyclotron times. Furthermore, this comparison allows us to evaluate the parameter α for this cusp. The quantity αP^3 in the local representation corresponds to $Pt_N/2m$ in the global representation, so

$$\alpha=t_N/2mP^2. \tag{5.6a}$$

Again presuming that the tip of the cusp is not far from the origin, then t_N is close to the return time of the parallel orbit to the origin,

$$t_N\simeq t_\parallel=2P/eF_0$$

and

$$\alpha\simeq(meF_0P)^{-1}. \tag{5.6b}$$

All of the same results, including the evaluation of α, can also be derived by comparing the parametric forms of the action $\widetilde{S}(t-t_N,\theta_{\rm out})\leftrightarrow\widetilde{S}(t',\theta')$ or the Jacobian $\widetilde{J}(t-t_N,\theta_{\rm out})\leftrightarrow\widetilde{J}(t',\theta')$, always presuming that z_c is not too far from the origin and $\theta_{\rm out}$ is small.

One more property of the returning orbits will be needed later. Locally the characteristic function associated with the returning orbits $\widetilde{S}(t,\theta_{\rm out})$ can be reexpressed in the canonical representation as $\widetilde{S}(p,z)$. We need the second derivative of this function at that value of p corresponding to the newly bifurcated orbit that returns to the origin. Noting that $\rho(p,z)=|\partial\widetilde{S}(p,z)/\partial p|$ [Eq. (4.4)], we propose that

$$\frac{\partial^2\widetilde{S}(p,z)}{\partial p^2}=-\frac{\partial\rho(p,z)}{\partial p}=\left(\frac{N\pi}{m\omega_L}\right)\tan^2\theta_{\rm out}. \tag{5.7}$$

Proof: From Eq. (4.1b), with $p_\rho=p$ close to the origin,

$$\rho=(p/m\omega_L)|\sin\omega_L t|, \tag{5.8a}$$

$$\left(\frac{\partial\rho}{\partial p}\right)_z=\frac{|\sin\omega_L t|}{m\omega_L}+\frac{p}{m}\cos(\omega_L t)\left(\frac{\partial t}{\partial p}\right)_z, \tag{5.8b}$$

$$\left(\frac{\partial t}{\partial p}\right)_z=-\frac{(\partial z/\partial p)_t}{(\partial z/\partial t)_p}=-\frac{(t/m)(\partial p_z/\partial p)}{p_z/m}=-\frac{tp}{p_z^2}. \tag{5.8c}$$

Now set $t=N\pi/\omega_L$,

$$\left(-\frac{\partial\rho}{\partial p}\right)_z=\frac{t}{m}\frac{p^2}{p_z^2}=\frac{N\pi}{m\omega_L}\tan^2\theta, \tag{5.9}$$

where θ is the returning angle of the orbit and is equal to the outgoing angle of the orbit.

Equation (5.7) will be used later in a stationary-phase evaluation of an integral.

B. The mixed-space outgoing wave

Continuing our evaluation of the quantities that go into the wave function (4.9) we now need the wave function on an initial surface, $\tilde{\Psi}(p_{x_0},p_{y_0},z_0)$. For this purpose we use a Fourier transform of the initial outgoing wave.

In configuration space, that initial outgoing wave was shown to be [paper I, Eq. (A11)]

$$\Psi_{\text{out}}(x,y,z)\sim(2im/\hbar^2)I_{\mathscr{l}}(k)\chi(\theta,\varphi)\exp(ikr)/r. \tag{5.10}$$

This formula describes the outgoing wave at distances r about $5a_0-100a_0$: large enough that the asymptotic form of the Hankel function is appropriate, but small enough that the curvature of the orbits caused by the external fields is negligible.

Let us take a surface $z=z_0$ somewhere in this vicinity (we might choose $z_0\sim20a_0$; it will drop out later anyway), and evaluate the mixed-space wave function on this surface,

$$\tilde{\Psi}(p_{x_0}p_{y_0}z_0)=(2\pi i\hbar)^{-1}\int\exp[-i(p_{x_0}x+p_{y_0}y)/\hbar]\times\Psi(x,y,z_0)dx\,dy. \tag{5.11}$$

Cartesian coordinates and a two-dimensional stationary-phase approximation are suitable:

$$(2\pi i\hbar)^{-1}\int_{-\infty}^{\infty}A(x,y)\exp[i\Phi(x,y)/\hbar]dx\,dy$$
$$\simeq(2\pi i\hbar)^{-1}A(x_0y_0)\exp[i\Phi(x_0y_0)/\hbar]\,\frac{(2\pi\hbar)}{|\det\Phi''|^{1/2}}\times\exp\left(i\,\frac{\pi}{4}\,\text{sgn}\Phi''\right), \tag{5.12}$$

where Φ'' is the matrix of second derivatives of $\Phi(x,y)$, $\det\Phi''$ is its determinant, and $\text{sgn}\Phi''$ is its signature (the number of positive eigenvalues minus the number of negative eigenvalues), all these quantities being evaluated at the stationary-phase point, (x_0,y_0). A straightforward calculation gives

$$\tilde{\Psi}(p_{x_0},p_{y_0},z_0)=(2im/\hbar^2)I_{\mathscr{l}}(k)\,\frac{\chi(\theta_p\varphi_p)}{P\,\cos\theta_p}\times\exp[ip_z(p_{x_0},p_{y_0})z_0/\hbar], \tag{5.13}$$

where (θ_p,φ_p) are polar and azimuthal angles in momentum space. As stated earlier, this formula holds for any z_0 between about $5a_0$ and $100a_0$, and for classically allowed (p_{x_0},p_{y_0}) (such that $p_{x_0}^2+p_{y_0}^2<P^2$).

C. Returning wave function

To calculate the complete returning wave function in the vicinity of the origin (when the cusp is near the origin), we also need the ratio of Jacobians. The absolute value of that ratio is equal to 1. Proof: For short times, the exact equation of motion (5.1) reduces to free-particle motion,

$$z(t,\theta_{\text{out}})\sim Pt\,\cos\theta_{\text{out}}/m,$$
$$p(t,\theta_{\text{out}})\sim P\,\sin\theta_{\text{out}} \tag{5.14}$$

so evaluation of the Jacobian (4.5a) gives

$$|J(p_{x_0}p_{y_0}z_0)|=p_0P^2\cos^2\theta_{\text{out}}/m=p_0p_{z0}^2/m \tag{5.15}$$

but for any orbit that returns to the origin $p_0=p$ and $p_{z0}=p_z$. Q.E.D.

Finally, the phase of the wave function in Eq. (4.9) is obtained by taking the relevant integrals

$$\tilde{S}=\int p_z dz-x dp_x-y dp_y$$

from the initial surface $z=z_0$ to the final point. Clearly we should combine that integral with the phase $p_z z_0$ in Eq. (5.13) and call the whole thing $\tilde{S}$. Let us evaluate that quantity at the cusp point:

$$\begin{aligned}\tilde{S}_c&=\tilde{S}(p_x=0,\ p_y=0,\ z=z_c)\\&=p_z(p_x,p_y)z_0+\int_{z_0}^{z_c}p_z dz-x\,dp_x-y\,dp_y\\&=\int_0^{z_c}[p_z(t,\theta_{\text{out}}=0)dz(t,\theta_{\text{out}}=0)/dt]dt\\&=S(x=0,\ y=0,\ z=z_c)=S_c.\end{aligned} \tag{5.16}$$

This integral from zero to z_c means along the parallel orbit from origin to turning point and back to the cusp point.

Then the phase of the returning wave is given by this value at the cusp point plus the local form, for which various representations were given in Eq. (4.3). Comparison of Eqs. (4.3e) and (5.16) gives the physical interpretation of $\tilde{S}_0=\tilde{S}_c+Pz_c$: it is the action of the parallel orbit from origin to origin,

$$\tilde{S}_0 = S_\parallel = \oint [p_z(t,\theta_{\text{out}}=0)dz(t,\theta_{\text{out}}=0)/dt]dt. \tag{5.17}$$

Combining all the above in Eq. (4.9), we obtain

$$\tilde{\Psi}(p_x p_y z) = (2im/\hbar^2) I_{\ell}(k) \frac{\chi(\theta_p,\varphi_p)}{P\cos\theta_p} e^{-i\nu\pi/2} \times \exp[i\tilde{S}(p,z)/\hbar]. \tag{5.18}$$

For z-polarized light, $\chi(\theta_p) = (4\pi)^{-1/2}\cos(\theta_p)$, and, following the same steps that were used to obtain Eq. (4.13), the returning wave is

$$\Psi_{\text{ret}}(\rho,z) = \tilde{B}\int_0^\infty J_0(p\rho/\hbar)\exp[i\tilde{S}(p,z)/\hbar]\frac{\chi(\theta_p)}{\cos\theta_p} p\, dp, \tag{5.19a}$$

$$\tilde{B} = -\left(\frac{2m}{\hbar^3 P}\right) I_{\ell}(k) e^{-i\nu\pi/2}. \tag{5.19b}$$

We have obtained precisely the local wave function for the focused cusp, now with all constants evaluated.

D. Photodetachment cross section

To obtain the photodetachment cross section we need the overlap of this returning wave with the source function $\langle D\psi_i|\psi_{\text{ret}}\rangle$. This quantity is an integral over the spatial variables ρ,z, involving the wave function ψ_{ret}, which is an integral over p. The result comes out very simply if we interchange the order of integration, integrating over ρ and z first, making use of a partial-wave expansion.

For this purpose, we separate $\tilde{S}(p,z)$ as in Eq. (4.3c),

$$\langle D\psi_i|\psi_{\text{ret}}\rangle = \tilde{B}\int dp\, \frac{\chi(\theta_p)}{\cos\theta_p} p\, \exp[i\tilde{S}(p,0)/\hbar]\int r^2 dr \times \sin\theta\, d\theta\, d\varphi r\, \cos\theta R(r) J_0(p\rho/\hbar) e^{ip_z(p)z}. \tag{5.20}$$

The partial-wave expansion (I.A22) [this notation denotes Eq. (A22) of paper I] can be used again,

$$J_0(p\rho/\hbar)e^{ip_z(p)z/\hbar} = (2\pi)\sum_{\ell} 2(-i)^{\ell} j_{\ell}(kr) Y_{\ell 0}(\theta,\varphi) \times Y^*_{\ell 0}(\theta_p\varphi_p). \tag{5.21}$$

The only difference between this formula and the one used in Eq. (I.A22) is that now the angles $\theta_p\varphi_p$ lie inside an integral. After integration over θ and φ, only the term having $\ell = 1$ survives, and it reduces to an old friend, Eq. (I.A7),

$$\int_0^\infty r^2 dr\, \sin\theta\, d\theta\, d\varphi r\, \cos\theta R(r) J_0(p\rho) e^{ip_z(p)z/\hbar} = (-4\pi i) I_1(k) \chi^*(\theta_p) \tag{5.22}$$

so

$$\langle D\psi_i|\psi_{\text{ret}}\rangle = \tilde{B}(-4\pi i) I_1(k)\int_0^\infty \exp[i\tilde{S}(p,0)/\hbar] \times \frac{|\chi(\theta_p)|^2}{\cos\theta_p} p\, dp. \tag{5.23}$$

At last we combine this formula with all the constants contained in Eq. (I.2.2) and simplify using (I.A10a):

$$\sigma_{\text{ret}} = \sigma_0\left(\frac{6\pi}{mE}\right)\text{Im}\left\{ie^{-i\nu\pi/2}\int_0^\infty \exp[i\tilde{S}(p,0)/\hbar] \times \frac{\chi^2(\theta_p)}{\cos\theta_p} p\, dp\right\}. \tag{5.24}$$

For numerical calculation of the cross section near the bifurcation we may use the representation (4.3d) for $\tilde{S}(p,0)$ and replace $\chi^2(\theta_p)/\cos\theta_p \simeq 1/4\pi$. Changing variables to $\epsilon = p^2/2$ we obtain

$$\sigma_{\text{ret}} = \sigma_0\left(\frac{6\pi}{mE}\right)\text{Im}\left\{i\, \exp i\left(S_\parallel/\hbar - \nu\frac{\pi}{2}\right) \times \left(\frac{1}{4\pi}\right)\int_0^\infty \exp\left[i/\hbar\left(\alpha\epsilon^2 - \frac{z_c}{P}\epsilon\right)\right]d\epsilon\right\} \tag{5.25a}$$

$$= \sigma_0\left(\frac{3}{2mE}\right)\text{Im}\left\{i\, \exp i\left(S_\parallel/\hbar - \nu\frac{\pi}{2}\right) \times F_1(-z_c/P(\hbar\alpha)^{1/2})\right\}. \tag{5.25b}$$

This is the formula we used in our numerical calculations.

E. Maslov indices and consistency check

Only one thing remains. We have not yet specified the value of ν. General theory [12,13] gives rules for calculating the value of ν from the properties of the complete Lagrangian manifold. Those rules correspond to the following prescription: ν must be chosen such that stationary-phase transformation of the wave function from (p_x, p_y) to (x,y) gives the correct μ for each orbit. The result of this analysis is that

$$\nu = \mu(\text{parallel orbit before bifurcation}) \tag{5.26a}$$

$$= \mu(\text{new orbit after bifurcation}) \tag{5.26b}$$

$$= \mu(\text{parallel orbit after bifurcation}) - 2. \tag{5.26c}$$

We can verify this and also provide a consistency check on our calculations by comparing Eq. (5.25) with the semiclassical formulas derived in the preceding paper. Let us apply the approximation (4.15a) to the integral (5.24), and consider only the stationary-phase term, keeping p as the variable of integration,

$$\sigma_{\rm ret}=\sigma_0\left(\frac{6\pi}{mE}\right)\mathrm{Im}\left\{ie^{-i\nu\pi/2}\left|\frac{2\pi\hbar}{\tilde{S}''(\hat{p},0)}\right|^{1/2}\frac{\chi^2(\hat{\theta}_p)}{\cos\hat{\theta}_p}\times\hat{p}\,\exp i\left(\tilde{S}(\hat{p},0)/\hbar+\frac{\pi}{4}\,\mathrm{sgn}S''(\hat{p})\right)\right\}. \quad (5.27a)$$

We already explained that the stationary-phase point $\hat{p}=P\sin\hat{\theta}_p$ corresponds to the new orbit, so $\tilde{S}(\hat{p},0)$ is the action around that orbit from origin to origin. Furthermore, we evaluated $\tilde{S}''(\hat{p},0)$ in Eqs. (5.7) and (5.8), and we note that this quantity is positive for the returning orbit. Therefore, combining and simplifying,

$$\sigma_{\rm ret}=\sigma_0 12\pi\left(\frac{\hbar\omega_L}{NE}\right)^{1/2}\chi^2(\theta_N)\sin\left[\frac{\tilde{S}_N}{\hbar}-(\nu-1)\,\frac{\pi}{2}+\frac{\pi}{4}\right] \quad (5.27b)$$

$$=\sigma_0 12\pi\left(\frac{\hbar\omega_L}{NE}\right)^{1/2}\chi^2(\theta_N)\sin(-)\left[\frac{\tilde{S}_N}{\hbar}-\nu\,\frac{\pi}{2}-\frac{\pi}{4}\right]. \quad (5.27c)$$

This is exactly Eq. (B28b) of the preceding paper, and it verifies Eq. (5.26b).

Similarly we can show that the end point contributions in Eq. (4.15a) or (4.15c) give Eq. (I.B28a), which we rewrite using

$$t_\parallel\simeq t_N+\frac{mz_c}{P} \quad (5.28)$$

as

$$\sigma_{\rm ret}=\sigma_0\,\frac{3\hbar}{|Pz_c|}\,\sin\left(-S_0+\mu_0\,\frac{\pi}{2}\right). \quad (5.29)$$

Before the bifurcation $z_c<0$, and applying Eq. (4.15c) to Eq. (5.25a) we find

$$\sigma_{\rm ret}=\sigma_0\,\frac{3}{2mE}\,\mathrm{Im}\left[ie^{i(S_0-i\nu\pi/2)}\,\frac{i\hbar}{(-z_c/P)}\right] \quad (5.30a)$$

$$=\sigma_0\,\frac{3\hbar}{|Pz_c|}\,(-)\sin\left[S_0-\nu\,\frac{\pi}{2}\right], \quad (5.30b)$$

which is precisely Eq. (I.B28a) with Eq. (5.26a). After the bifurcation, Eq. (5.30a) still holds, but $-z_c$ is negative, so we obtain

$$\sigma_{\rm ret}=\sigma_0\,\frac{3\hbar}{|Pz_c|}\,(-)\sin\left(\frac{S_0}{\hbar}-(\nu-2)\,\frac{\pi}{2}\right), \quad (5.31)$$

which verifies Eq. (5.26c), and gives yet another proof that the Maslov index of the parallel orbit increases by 2 on passage through the focused cusp.

VI. CONCLUSION

We have derived Eqs. (5.25), a semiclassical formula for the photodetachment cross section in the vicinity of a bifurcation of the parallel orbit. We already saw in Fig. 1 that this formula compares well with a quantum calculation in the vicinity of the fourth bifurcation. At present, no experiments on this system are available for comparison.

In the next paper, we examine photoexcitation of a neutral atom in an electric field. Similar bifurcations occur, but the theory also has to contend with the Coulomb singularity. We find that analogous formulas correct the divergences in the semiclassical approximation, and we compare the results with measured recurrence spectra.

ACKNOWLEDGMENTS

This research was supported by the National Science Foundation (JILA, WVU, and W&M), the Office of Naval Research (W&M), and by Research Corporation and the Petroleum Research Fund (Kean).

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[7] To make the theory rigorous, the Fourier integral is restricted to a local domain of $\mathbf{q}_\beta$ space, using a smooth cutoff function.

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[10] In general, a Lagrangian manifold has a good projection into at least one of the four ''Lagrangian coordinate planes'' (x,z), (p_x,z), (x,p_z), or (p_x,p_z). For each acceptable plane there is a generator whose derivatives define the manifold according to canonical formulas analogous to Eq. (3.2). The generator must therefore satisfy the relevant Hamilton-Jacobi equation. The assertion here is that the (p_x,z) representation is the relevant one.

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