Orbit-averaged quantities, the classical Hellmann-Feynman theorem, and the magnetic flux enclosed by gyro-motion

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Action integrals are often used to average a system over fast oscillations and obtain reduced dynamics. It is not surprising, then, that action integrals play a central role in the Hellmann-Feynman theorem of classical mechanics, which furnishes the values of certain quantities averaged over one period of rapid oscillation. This paper revisits the classical Hellmann-Feynman theorem, rederiving it in connection to an analogous theorem involving the time-averaged evolution of canonical coordinates. We then apply a modified version of the Hellmann-Feynman theorem to obtain a new result: the magnetic flux enclosed by one period of gyro-motion of a charged particle in a non-uniform magnetic field. These results further demonstrate the utility of the action integral in regards to obtaining orbit-averaged quantities and the usefulness of this formalism in characterizing charged particle motion. © *2015 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4905635]

I. INTRODUCTION

Many systems of interest exhibit a separation of time scales in that one aspect of motion occurs on a much shorter timescale compared to the rest of the system. It is often desirable to obtain reduced dynamics by averaging over the fast oscillations, and in Hamiltonian mechanics this can be realized by the use of action integrals [Ref. 1, Sec. 10.6]. The archetypal example in plasma physics is charged particle motion in magnetic fields, where the action integral associated with the fast gyro-motion, the adiabatic invariant, μ, plays a central role in the guiding center theory approximation where gyro-motion is averaged out. Applications of guiding center theory are diverse and range from particle confinement in the Earth's magnetosphere[2] and in solar coronal loops[3] to the pinch effect in tokamaks.[4–8] Even for non-adiabatic phenomena, such as large energy transfer to particles interacting with electromagnetic waves,[9–11] the introduction of the action integral and its conjugate angle variable is extremely useful, and applications also exist beyond particle motion, such as in conservation laws for waves, including interactions between discrete and continuum modes.[12]

Use of the action integral typically implies that the system has been averaged over the fast variation, and this feature of the action integral is born out in the adaptation of the Hellmann-Feynman theorem for classical mechanics[13,14] (see Ref. 15 for a historical account), which furnishes the time-averaged values of certain terms in the Hamiltonian once the action integral has been introduced. Let $H(q,p,\lambda)$ be a Hamiltonian system with parameter λ, and let $J=\oint p dq$ denote the action integral of this system. As will be explained in Sec. II, H can be written as a function of J and λ, and we let $\tilde{H}(J,\lambda)$ denote this functional form. The classical Hellmann-Feynman theorem states that

$$\frac{\partial \tilde{H}}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle, \tag{1}$$

where $\langle \ldots \rangle$ denotes a time average over one period Δt. Equation (1) can be used to derive the average values of various quantities of physical interest using the functional form of $\tilde{H}$. For example, a harmonic oscillator has the Hamiltonian $H = p^2/2m + m\omega^2 q^2/2$ and $\tilde{H} = \omega J/2\pi$. Applying the classical Hellmann-Feynman theorem to the parameter ω gives $\langle q^2 \rangle = J/2\pi m\omega$. The Hellmann-Feynman theorem was originally formulated for quantum mechanics[16–18] and states that

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \middle| \frac{\partial \hat{H}}{\partial \lambda} \middle| \psi_n \right\rangle, \tag{2}$$

where $|\psi_n\rangle$ is the nth eigenstate of the Hamiltonian operator $\hat{H}$ and E_n is the energy associated with this eigenstate. For the quantum harmonic oscillator, $\hat{H} = (1/2m)\hat{p}^2 + (m\omega^2/2)\hat{q}^2$ and $E_n = \hbar\omega(n+1/2)$, so applying Eq. (2) to the parameter ω gives $\langle q^2 \rangle = (n+1/2)\hbar/\omega m$. The classical version of the theorem is often viewed as a limit of the quantum version. Indeed, McKinley's derivation,[13] which holds $\oint p dq$ constant under a particular class of variations, comes from Schwinger's variational formulation of quantum mechanics[19] extrapolated to the classical limit. Also, Susskind applies the results from the quantum version of the theorem to the analogous classical system in the limit $\hbar \to 0$.[20] In general, there is a large body of work exploiting the quantum version of the theorem to develop analytical solutions to various perturbation problems,[21–24] but less attention has been given to the classical version.

The purpose of this paper is two-fold. First, we present an alternate derivation of the classical Hellman-Feynman theory. This derivation exploits the formalism of Ref. 25, where the average evolution of phase space coordinates is derived via the action integral. This proof highlights the similarities between system parameters and conserved canonical

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momenta. Second, we apply a modified version of Eq. (1) to derive a result which, to our knowledge, has not appeared in the literature: the calculation of the magnetic flux enclosed by a gyro-orbit of a charged particle in a non-uniform magnetic field using the action integral. The derivation factors out the drift motion and gives the flux in the drift frame of the particle. The formula derived is verified for two non-trivial cases; in each case, the flux derived is exact, as the methodology does not resort to approximating the magnetic field as uniform nor the Larmor orbits as perfectly circular motion.

II. DERIVATION OF THE CLASSICAL HELLMANN-FEYNMAN THEOREM

Let $H(\xi,P_\xi,\lambda)$ be a Hamiltonian system with parameter λ and coordinate ξ that is oscillatory with period Δt. The action integral J is a function of H and λ

$$J(H,\lambda)=\oint P_\xi(H,\xi,\lambda)d\xi. \tag{3}$$

Our first claim is that

$$\frac{\partial J}{\partial \lambda}=-\int_{t_0}^{t_0+\Delta t}\frac{\partial H}{\partial \lambda}dt. \tag{4}$$

To prove Eq. (4), we first note that

$$\frac{\partial J}{\partial \lambda}=\oint\frac{\partial P_\xi(H,\xi,\lambda)}{\partial \lambda}d\xi \tag{5}$$

because there is no contribution from differentiating the integral bounds since the contour of integration in the ξP_ξ plane is closed for a time-independent Hamiltonian. Next, we have

$$\frac{\partial P_\xi}{\partial \lambda}=-\frac{\partial H/\partial \lambda}{\partial H/\partial P_\xi}, \tag{6}$$

which follows from the differential of $H(\xi,P_\xi,\lambda)$

$$dH=\frac{\partial H}{\partial \xi}d\xi+\frac{\partial H}{\partial P_\xi}dP_\xi+\frac{\partial H}{\partial \lambda}d\lambda, \tag{7}$$

after setting $dH=0$ and $d\xi=0$. Finally, using Eq. (6) in Eq. (5) and then invoking Hamilton's equations give

$$\frac{\partial J}{\partial \lambda}=-\oint\frac{\partial H/\partial \lambda}{\partial H/\partial P_\xi}d\xi \tag{8}$$

$$=-\oint\frac{\partial H/\partial \lambda}{d\xi/dt}d\xi=-\int_{t_0}^{t_0+\Delta t}\frac{\partial H}{\partial \lambda}dt, \tag{9}$$

which proves Eq. (4).

We now derive Eq. (1) from Eq. (4). Note that Eq. (4) is closely related to the well-known result

$$\frac{\partial J}{\partial H}=\oint\frac{\partial P_\xi}{\partial H}d\xi=\oint\frac{1}{\partial H/\partial P_\xi}d\xi=\oint\frac{1}{d\xi/dt}d\xi=\Delta t. \tag{10}$$

To obtain a time average of the quantity $\partial H/\partial\lambda$, we use Eq. (4) and then Eq. (10) to write

$$\left\langle\frac{\partial H}{\partial \lambda}\right\rangle=\frac{1}{\Delta t}\int_{t_0}^{t_0+\Delta t}\frac{\partial H}{\partial \lambda}dt=-\frac{\partial J/\partial \lambda}{\partial J/\partial H}. \tag{11}$$

Let $\tilde H=\tilde H(J,\lambda)$ be the Hamiltonian written as a function of J and λ rather than ξ, P_ξ, and λ; one obtains $\tilde H$ by inverting $J=J(H,\lambda)$ for H. All that remains to prove Eq. (1) is to show that

$$-\frac{\partial J/\partial \lambda}{\partial J/\partial H}=\frac{\partial \tilde H}{\partial \lambda}, \tag{12}$$

which we prove by analyzing the differential $dJ(H,\lambda)$

$$dJ=\frac{\partial J}{\partial H}dH+\frac{\partial J}{\partial \lambda}d\lambda, \tag{13}$$

upon setting $dJ=0$. Note that $dH=d\tilde H$ since H and $\tilde H$ are two different functional forms for the same quantity. Also, since the differentials hold J constant ($dJ=0$), we have $d\tilde H/d\lambda=\partial\tilde H/\partial\lambda$. Note that for such variations $dH/d\lambda \neq \partial H/\partial\lambda$ since the latter implies that ξ and P_ξ are being held constant. This proves Eq. (13) and hence Eq. (1). In both Refs. 13 and 14, the link between holding the abbreviated action constant and the Hellmann-Feynman theorem is not presented, in general, but is only shown explicitly for certain Hamiltonians. The above proof is general for any functional form of H.

The above proof is based on the formalism presented in Ref. 25, and it is insightful to compare the two. In Ref. 25, a two-dimensional Hamiltonian system was considered involving an ignorable coordinate η and an associated conserved momentum P_η. Over the course of one cycle of ξ motion, the coordinate η evolved by an amount $\Delta\eta$, and it was shown that

$$\Delta\eta=-\frac{\partial J}{\partial P_\eta}\quad \frac{\Delta\eta}{\Delta t}=\frac{\partial \tilde H}{\partial P_\eta}, \tag{14}$$

where in this case $\tilde H=\tilde H(J,P_\eta)$. It is clear that the parameter λ and the conserved momentum P_η play analogous roles in the two cases. This is not too surprising, as ignorable coordinates do not appear in the Hamiltonian, and their conjugate canonical momenta are conserved and can be regarded as parameters of the Hamiltonian rather than as dynamic variables. The converse is also true: given a parameter λ, we can regard λ as the conserved canonical momentum conjugate to some artificially introduced ignorable phase space coordinate. Indeed, one could derive Eqs. (1) and (4) from Eq. (14) by starting with the system $H(\xi,P_\xi,\lambda)$ and promoting λ to a conserved momentum conjugate to a fictitious ignorable coordinate χ so that, from Eq. (14),

$$\Delta\chi=-\frac{\partial J}{\partial \lambda}, \tag{15}$$

but also

$$\Delta\chi=\int_{t_0}^{t_0+\Delta t}\dot\chi dt=\int_{t_0}^{t_0+\Delta t}\frac{\partial H}{\partial \lambda}dt, \tag{16}$$

proving Eq. (4) from Eq. (14).

Although derived in the context of time-independent systems with exactly periodic trajectories, Eq. (1) is accurate to lowest-order in time-dependent systems when the explicit time-dependence is slow enough that the motion is nearly periodic. That is, suppose $\lambda(t) \approx \lambda_0 + \delta\lambda(t)$ with λ_0 constant in time and $\epsilon = \delta\lambda/\lambda_0 \ll 1$. Then, to first order

$$H(q,p,\lambda) \approx H(q,p,\lambda_0) + \delta\lambda \frac{\partial H}{\partial \lambda}. \tag{17}$$

The first term describes the unperturbed evolution of the system, while the second term can be considered a small perturbation. We consider the evolution over a single period of motion; the trajectories for q and p will then, in the absence of resonances, follow the unperturbed trajectories plus a small first-order correction, e.g., $q(t) \approx q_0(t) + \epsilon q_1(t)$ and $p(t) \approx p_0(t) + \epsilon p_1(t)$. Then, in computing the average of any phase-space function $f(q,p,\lambda)$ over a period of motion, the averaging will be equal to its unperturbed value plus some correction of first order

$$\frac{1}{T}\int_0^T f(q(t),p(t),\lambda(t))dt \approx \frac{1}{T}\int_0^T f(q_0(t),p_0(t),\lambda_0)dt + O(\epsilon). \tag{18}$$

Finally, if f is chosen to be $\partial H/\partial\lambda$, the unperturbed value is precisely that computed in Eq. (1), as it results from "freezing" the slowly varying parameter and integrating along the unperturbed orbit. Also, any changes to the period of motion are of order ϵ, so that any changes to the averaging due to changing the bounds of integration are also first order. Thus, for systems with slowly varying parameters in the absence of resonances, the exact average $\langle \partial H/\partial\lambda\rangle$ over a single period is equal to the averaging performed at fixed λ plus first-order corrections, and the averaging at fixed λ is given by the Hellmann-Feynman theorem to be $\partial\tilde{H}/\partial\lambda$. One could compute the first-order corrections using perturbation theory [Ref. 26, Chap. 2], but such small corrections are not the focus of this paper. Section III contains a time-dependent example, in which Eq. (1) holds quite accurately.

III. EXAMPLE: PENNING TRAP

In this section, we use the ideal Penning trap[27,28] to demonstrate the classical Hellmann-Feynman theorem in a time-dependent situation. The calculations performed here will also be used in Appendix B to compute the magnetic flux through a gyro-orbit of a particle confined in the trap. An ideal Penning trap consists of a uniform axial field $\mathbf{B} = B_0\hat{z}$ (so $\mathbf{A} = (1/2)rB_0\hat{\theta}$) superimposed with the potential

$$V = \frac{1}{2}\frac{m}{q}\omega_z^2\left(z^2 - \frac{1}{2}r^2\right). \tag{19}$$

The Hamiltonian is

$$H = \frac{P_r^2}{2m} + \frac{\left(P_\theta - qB_0r^2/2\right)^2}{2mr^2} + \frac{P_z^2}{2m} + \frac{1}{2}m\omega_z^2\left(z^2 - \frac{1}{2}r^2\right). \tag{20}$$

We treat r as the rapidly oscillating variable; note that the axial motion is completely decoupled from the radial motion. The action integral J, for particles whose gyro-orbits do not encircle the axis, is derived in Appendix A and takes the form

$$J = 2\pi\left[\frac{\Omega_-}{\Omega_r}P_\theta + \frac{H - P_z^2/2m - (m/2)\omega_z^2z^2}{\Omega_r}\right], \tag{21}$$

where we have defined $\Omega_r = \sqrt{\Omega_c^2 - 2\omega_z^2}$ and $\Omega_- = (\Omega_c - \Omega_r)/2$ with $\Omega_c = qB_0/m$. From Eq. (10), Ω_r is the angular frequency of the radial motion. As discussed in Appendix A, this radial frequency differs from the modified cyclotron frequency $\Omega_+ = (\Omega_c + \Omega_r)/2$. Ω_- is known as the magnetron frequency and is the frequency of the azimuthal motion, since application of Eq. (14) gives

$$\Delta\theta = -\frac{\partial J}{\partial P_\theta} = -2\pi\frac{\Omega_-}{\Omega_r} \tag{22}$$

and thus

$$\frac{\Delta\theta}{\Delta t} = -\Omega_-. \tag{23}$$

The average value of r^2 can be obtained as follows. From Eq. (21), we have

$$\tilde{H} = \frac{\Omega_r}{2\pi}J - \Omega_- P_\theta + \frac{1}{2m}P_z^2 + \frac{m}{2}\omega_z^2z^2. \tag{24}$$

It is straight-forward to show that

$$\left\langle\frac{\partial H}{\partial\omega_z}\right\rangle = m\omega_z\left(z^2 - \frac{1}{2}\langle r^2\rangle\right), \tag{25}$$

$$\frac{\partial\tilde{H}}{\partial\omega_z} = -\frac{1}{\pi}\frac{\omega_z}{\Omega_r}J - \frac{\omega_z}{\Omega_r}P_\theta + m\omega_z z^2. \tag{26}$$

Equating the two quantities, as per Eq. (1), gives

$$\langle r^2\rangle = \frac{2J/\pi + 2P_\theta}{m\Omega_r}. \tag{27}$$

Numerical computations of the complete orbit show that this formula is correct even when the magnetic field is allowed to vary in time; see Fig. 1. From Eq. (27), we have $\pi\langle r^2\rangle\Omega_r = (2J + 2\pi P_\theta)/m$, so, if the Penning trap is slowly changed in an adiabatic and axisymmetric fashion, then $\pi\langle r^2\rangle\Omega_r$ is an adiabatic invariant even though both $\langle r^2\rangle$ and Ω_r vary. Note that $\pi\langle r^2\rangle$ is the area of the circle traced out by the magnetron motion. If we then define a modified magnetic field strength $B_m = \sqrt{B_0^2 - 2\omega_z^2m^2/q^2} = m\Omega_r/q$, then the modified flux through the magnetron orbit, $\pi\langle r^2\rangle B_m$, is adiabatically invariant. This is not true of the ordinary magnetic flux $\pi\langle r^2\rangle B_0$.

IV. MAGNETIC FLUX ENCLOSED BY GYRO-MOTION

With judicious choices of parameters, the Hellmann-Feynman theorem can be used to glean useful properties of the averaged system.[13] In this section, we demonstrate a new application of the theory: for a particle of charge q in a magnetic field, differentiating J with respect to q is

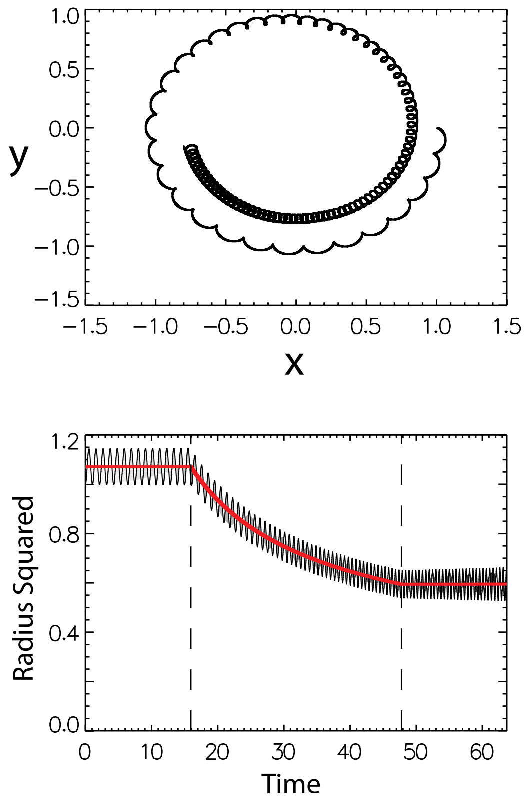

FIG. 1. (Top) A particle orbit in a Penning trap with a time-varying magnetic field. As magnetic field ramps up linearly, the magnetron orbit contracts in radius. (Bottom) The thin curve is the computed value of r^2 plotted as a function of time, whereas the thick line is the value of $\langle r^2 \rangle$ given by Eq. (27). One can verify that Eq. (27), derived from the Hellmann-Feynman theorem, tracks the computed value very well even in this time-dependent case. The dashed vertical lines indicate the onset and end of the linear magnetic field ramp; the field doubles in value during this time.

related to the magnetic flux enclosed by a gyro-orbit. This flux is previously only computed by approximating the particle motion as circular Larmor orbits and approximating the magnetic field as uniform, but the calculations presented here are exact and take into account the full trajectory and the non-uniformities of the magnetic field. Moreover, the calculations carefully account for the drift motion of the particle, giving the flux in the particle drift frame. The flux derived is verified numerically for two distinct and non-trivial examples: planar orbits outside a current-carrying wire and orbits in an ideal Penning trap (handled in Appendix B).

We first show the connection between $\partial J/\partial q$ and the flux enclosed by a gyro-orbit for a magnetic field, in which two Cartesian coordinates are ignorable. The more general case using generalized coordinates is handled in Appendix B. Using Eq. (4) and the Hamiltonian for charged particle motion,

$$H(\mathbf{x},\mathbf{P},q) = \frac{(\mathbf{P}-q\mathbf{A})^2}{2m} + qV, \tag{28}$$

we find that for an electromagnetic field that admits an adiabatic invariant of non-relativistic particle motion

$$\begin{aligned}\frac{\partial J}{\partial q} &= -\int_{t_0}^{t_0+\Delta t} \frac{\partial H(\mathbf{x},\mathbf{P},q)}{\partial q}dt \\ &= -\int_{t_0}^{t_0+\Delta t}\left[-\frac{\mathbf{P}-q\mathbf{A}}{m}\cdot\mathbf{A}+V\right]dt \\ &= -\int_{t_0}^{t_0+\Delta t}[-\mathbf{v}\cdot\mathbf{A}+V]dt, \qquad (29)\\ &= \int \mathbf{A}\cdot d\mathbf{l} - \int_{t_0}^{t_0+\Delta t} V dt. \qquad (30)\end{aligned}$$

The path integral in Eq. (30) is over one period of motion in the lab frame. If the trajectory were closed, we would have $\int \mathbf{A}\cdot d\mathbf{l} = \int \mathbf{B}\cdot d\mathbf{S}$. In the laboratory frame, the trajectory is typically not closed, but it is closed in the drift frame. We therefore proceed by splitting the motion into drift and oscillatory pieces. We denote the drift velocity as $\mathbf{v}_d = \Delta\mathbf{x}/\Delta t$, where $\Delta\mathbf{x} = -\partial J/\partial\mathbf{P}$ is the vector displacement over one period as given by Eq. (14). We then define the oscillatory velocity $\mathbf{v}'$ as $\mathbf{v}' = \mathbf{v}-\mathbf{v}_d$, so that $\mathbf{v}$ is the sum of drift and oscillatory parts. Further define $d\mathbf{l}' = \mathbf{v}'dt$. We then obtain

$$\begin{aligned}\frac{\partial J}{\partial q} &= \int_{t_0}^{t_0+\Delta t}\mathbf{A}\cdot(\mathbf{v}'+\mathbf{v}_d)dt - \int_{t_0}^{t_0+\Delta t} V dt, \qquad (31)\\ &= \oint \mathbf{A}\cdot d\mathbf{l}' + \int_{t_0}^{t_0+\Delta t}\mathbf{v_d}\cdot\mathbf{A}\,dt - \int_{t_0}^{t_0+\Delta t} V dt. \qquad (32)\end{aligned}$$

We identify the first integral as the magnetic flux Φ contained by the closed drift-frame trajectory. The second integral can be rewritten using $q\mathbf{A} = \mathbf{P}-m\mathbf{v}$. The quantity $\mathbf{P}\cdot\mathbf{v}_d$ is a constant of motion, as the drift $\mathbf{v}_d$ is in the direction of the ignorable Cartesian directions, so the canonical momenta along the drift direction is conserved, and $\mathbf{v}_d\cdot\mathbf{P}$ is therefore constant. Using this result, we obtain

$$\frac{\partial J}{\partial q} = \Phi + \frac{1}{q}(\mathbf{P}-m\mathbf{v}_d)\cdot\Delta\mathbf{x} - \int_{t_0}^{t_0+\Delta t} V dt. \tag{33}$$

Equation (33) is the desired relationship between flux and $\partial J/\partial q$. If there is a non-zero potential V, its average must be computed, e.g., via Eq. (12). The gauge invariance of Eq. (33) is demonstrated in Appendix C. Note that $\int \mathbf{A}\cdot d\mathbf{l}$ is related to the action for magnetic field lines[29] and also to the phase shift due to the Aharonov-Bohm effect,[30] so Eq. (30) could be of particular value in quantum systems.

We now compute the flux for several examples. For a charged particle in a uniform magnetic field $\mathbf{B} = B\hat{z}$ with a parallel momentum $P_z = mv_z$, the action integral is[25]

$$J = 2\pi\frac{m}{|q|}\frac{H-P_z^2/2m}{B}. \tag{34}$$

The absolute sign on q ensures that the period, $\Delta t = \partial J/\partial H$, is positive. From Eq. (33), we have

$$\begin{aligned}\Phi &= \frac{\partial J}{\partial q} - \frac{1}{q}(\mathbf{P} - m\mathbf{v}_d)\cdot\Delta\mathbf{x} \\ &= -\mathrm{sgn}(q)2\pi\frac{m}{q^2}\frac{H - P_z^2/2m}{B} \\ &= -\mathrm{sgn}(q)\pi\frac{m^2 v_\perp^2}{q^2 B} \\ &= -\mathrm{sgn}(q)\pi r_L^2 B.\end{aligned} \tag{35}$$

The term $(\mathbf{P} - m\mathbf{v}_d)\cdot\Delta\mathbf{x}$ vanishes because the only drift is in the z direction: $\mathbf{v}_d = (P_z/m)\hat{z}$. Note that Φ is negative for positive q and positive for negative q in accordance with the diamagnetism of particle orbits. Equation (35) is the expected result because for a uniform field the Larmor radius is $r_L = mv/|q|B$, and the flux is $\Phi = \pm\pi r_L^2 B$. Note also that $q\Phi = -J$, that is, the flux is proportional to the adiabatic invariant. We will soon see that this relationship is only valid in the limit of a uniform magnetic field and does not hold in general.

We now consider orbits in the magnetic field $\mathbf{B} = \mu_0 I/2\pi r\hat{\phi}$ in cylindrical coordinates. Such a magnetic field occurs outside current-carrying wires and inside toroidal solenoids. Charged particles with zero angular momentum about the z-axis will execute planar motion in a plane containing the z-axis. For such particles, the action is[25]

$$J = \mathrm{sgn}(q)2\pi R m v e^{-P_z/m\beta} I_1\left(\frac{v}{\beta}\right), \tag{36}$$

where R is an arbitrary length scale, m is the electron mass, v is the electron velocity, P_z is the canonical z-momentum, $\beta = \mu_0 I q/2\pi m$ is a characteristic velocity that depends on the wire current I and is positive for positive q and negative for negative q, and I_1 is a modified Bessel function. Using the identity $(xI_1(x))' = xI_0(x)$, it is seen that

$$\begin{aligned}\Delta z &= -\frac{\partial J}{\partial P_z} \\ &= \mathrm{sgn}(q)2\pi R\frac{v}{\beta}e^{-P_z/m\beta} I_1\left(\frac{v}{\beta}\right),\end{aligned} \tag{37}$$

$$\begin{aligned}\Delta t &= \frac{\partial J}{\partial H} = \frac{1}{mv}\frac{\partial J}{\partial v} \\ &= \mathrm{sgn}(q)2\pi\frac{R}{\beta}e^{-P_z/m\beta} I_0\left(\frac{v}{\beta}\right).\end{aligned} \tag{38}$$

Since I_1 is odd and I_0 is even, both J and Δt are positive for all q, while Δz is positive for positive q and negative for negative q. It is also seen that

$$\begin{aligned}\frac{\partial J}{\partial q} &= \frac{\beta}{q}\frac{\partial J}{\partial \beta} = sgn(q)2\pi\frac{mRve^{-P_z/m\beta}}{q} \\ &\times\left[\left(1 + \frac{P_z}{m\beta}\right)I_1\left(\frac{v}{\beta}\right) - \frac{v}{\beta}I_0\left(\frac{v}{\beta}\right)\right].\end{aligned} \tag{39}$$

Equation (33) then gives

$$q\Phi = J\left[1 - \frac{v}{\beta}\frac{I_0(v/\beta)}{I_1(v/\beta)} + \frac{v}{\beta}\frac{I_1(v/\beta)}{I_0(v/\beta)}\right]. \tag{40}$$

Numerical simulations of trajectories in their drift frames confirm that this formula is correct. It is apparent that $q\Phi \neq -J$, showing the magnetic flux enclosed by a gyro-orbit is distinct from the action integral. However, in the limit $v \ll \beta$ (for which $I_0(x) \approx 1$ and $I_1(x) \approx (1/2)x$ for small x), we do indeed recover $q\Phi \approx -J$.

In Sec. II, we noted that parameters and conserved canonical momenta play similar roles. In light of this comparison, we now note that q has previously been promoted to a canonical momentum. Kaluza[31] and Klein[32] proposed a five-dimensional spacetime model to unify gravity and electromagnetism, and in the five-dimensional Kaluza-Klein Lagrangian for a charged particle in the non-relativistic limit, the conserved momentum associated with the added dimension can be identified as the particle charge q [Ref. 33, Sec. 7.5].

V. ALTERNATE FORMULA FOR THE MAGNETIC FLUX

Section IV derived the magnetic flux enclosed by the gyro-motion by differentiating the action integral with respect to the particle charge. Here, we derive an alternate formula for the flux that does not involve $\partial J/\partial q$. For simplicity, we use Cartesian coordinates; a proof using generalized coordinates can be obtained using the machinery developed in Appendix B.

Suppose that the motion is periodic in one coordinate, say, x, and that the y and z coordinates are ignorable. We consider H as a function of the coordinates, momenta, and parameters q and m; that is, $H = H(\mathbf{x}, \mathbf{P}, q, m)$. From Eq. (28), H is a homogeneous function of degree one [Ref. 34, pg. 4] in the variables $\mathbf{P}$, q, and m

$$H(\mathbf{x}, \lambda\mathbf{P}, \lambda q, \lambda m) = \lambda H. \tag{41}$$

It follows that when $H = H(\mathbf{x}, \mathbf{P}, q, m)$ is solved for P_x, then P_x is a homogeneous function of degree one in the variables H, P_y, P_z, q, and m

$$P_x(\mathbf{x}, \lambda H, \lambda P_y, \lambda P_z, \lambda q, \lambda m) = \lambda P_x. \tag{42}$$

Then, J is also a homogeneous function of degree one in the variables H, P_y, P_z, q, and m

$$J(y, z, \lambda P_y, \lambda P_z, \lambda H, \lambda q, \lambda m) = \lambda J. \tag{43}$$

Applying Euler's theorem of homogeneous functions [Ref. 1, pg. 62] to J (i.e., differentiating with respect to λ and then setting $\lambda = 1$), we obtain

$$J = P_y\frac{\partial J}{\partial P_y} + P_z\frac{\partial J}{\partial P_z} + H\frac{\partial J}{\partial H} + m\frac{\partial J}{\partial m} + q\frac{\partial J}{\partial q} \tag{44}$$

or

$$J = -P_y\Delta y - P_z\Delta z + H\Delta t + m\frac{\partial J}{\partial m} + q\frac{\partial J}{\partial q}. \tag{45}$$

We reformulate the last two terms in this equation as follows. Using Eq. (4), we can relate $\partial J/\partial m$ to the kinetic energy KE of the particle, as in Ref. 13

$$m\frac{\partial J}{\partial m} = -m\int_{t_0}^{t_0+\Delta t}\frac{\partial H}{\partial m}dt = \int_{t_0}^{t_0+\Delta t}\mathrm{KE}\,dt = H\Delta t - \int_{t_0}^{t_0+\Delta t}V dt. \tag{46}$$

Also, using Eq. (33), we rewrite $\partial J/\partial q$ as

$$q\frac{\partial J}{\partial q} = q\Phi - P_y\frac{\partial J}{\partial P_y} - P_z\frac{\partial J}{\partial P_z} - mv_d^2\frac{\partial J}{\partial H}. \tag{47}$$

Using Eqs. (46) and (47) in Eq. (45), we obtain

$$J = q\Phi + 2\left(H - \frac{1}{2}mv_d^2\right)\Delta t, \tag{48}$$

an alternate formula for the flux Φ that involves J but not its derivative $\partial J/\partial q$. Again, we find that, in general, $q\Phi \neq -J$, but in the limit of a uniform magnetic field, for which $H - (1/2)mv_d^2 \approx (1/2)mv_\perp^2$ and $\Delta t \approx 2\pi m/qB$, we recover $q\Phi = -J$.

VI. CONCLUSIONS

The classical Hellmann-Feynman theorem was derived in relationship to an analogous theorem regarding the averaged evolution of phase-space coordinates. This highlights the comparable role of conserved canonical momenta and system parameters. The ideal Penning trap demonstrates an instance where the theorem can be applied accurately to a time-dependent situation. The Hellmann-Feynman theorem was then utilized in a novel application: to compute the flux enclosed by one period of gyro-motion. This flux is computed exactly for two non-trivial cases: planar orbits outside a current channel and orbits in an ideal Penning trap (Appendix B). The theorem further stresses that the key quantity when regarding the orbit-averaged or reduced system is the action variable associated with the periodic coordinate being averaged.

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APPENDIX A: ACTION INTEGRAL FOR THE IDEAL PENNING TRAP

The action integral for the radial motion in a Penning trap is obtained by first solving the Hamiltonian, Eq. (20), for P_r and then substituting into $J = \oint P_r dr$

$$J = \oint\sqrt{2mH_\perp + qB_0P_\theta - P_\theta^2/r^2 - m^2\Omega_r^2r^2/4}\,dr, \tag{A1}$$

where $H_\perp = H - P_z^2/2m - m\omega_z^2z^2/2$ is the energy in the xy plane and $\Omega_r = \sqrt{\Omega_c^2 - 2\omega_z^2}$ with $\Omega_c = qB_0/m$. To evaluate this integral, we use Sommerfeld's approach as outlined by Goldstein *et al.*,[1] which can be contrasted with the method of canonical transformation.[35] In the complex plane, the polynomial under the radical has four roots: the two radial turning points and their negatives. We introduce branch cuts between the pairs of turning points (see Fig. 2) such that we take the positive root above the cuts and the negative root below. The integral is then described by a contour that tightly encircles the right-hand branch cut in a clockwise sense (contour I). We can then deform the contour to a large circle (contour II) with the contour encircling the pole at $r = 0$ and the left-hand cut. The value of the contour around the left-hand cut is minus that around the positive cut, and the pole at $r = 0$ has a residue of $\sqrt{-P_\theta^2} = i|P_\theta|$. Therefore, we have

$$J = \oint_I P_r dr = -J + 2\pi i(i|P_\theta|) + \oint_{II} P_r dr. \tag{A2}$$

Along contour II, the integral approaches another integral of the form

$$\oint\sqrt{a^2 - b^2Z^2}dZ, \tag{A3}$$

with $a^2 = 2mH_\perp + qB_0P_\theta$ and $b = m\Omega_r/2$. This can be evaluated in closed form by standard means, e.g., deforming the contour closely around the branch cut between $Z = \pm a/b$ and using the substitution $\sin\theta = bZ/a$ such that

$$\int_{II}\sqrt{a^2 - b^2Z^2}dZ = \pi\frac{a^2}{b}. \tag{A4}$$

Using the result of Eq. (A4) in Eq. (A2) gives

$$J = -\pi|P_\theta| + 2\pi\left[\frac{H_\perp + P_\theta\Omega_c/2}{\Omega_r}\right]. \tag{A5}$$

The $|P_\theta|$ term is a feature of cylindrical geometry: assuming that qA_θ is positive; particles with positive P_θ have gyro-orbits that do not encircle the origin, whereas particles with negative P_θ do encircle the origin with their gyromotion. For non-encircling particles, $P_\theta > 0$ and $|P_\theta| = P_\theta$, so

$$J = 2\pi\frac{\Omega_-}{\Omega_r}P_\theta + 2\pi\frac{H_\perp}{\Omega_r}, \tag{A6}$$

with $\Omega_- = (\Omega_c - \Omega_r)/2$.

By applying Eq. (10) to Eq. (A6), Ω_r is seen to be the radial frequency of motion. Readers who are familiar with the theory of Penning traps will recognize that this radial frequency is not equal to the modified cyclotron frequency $\Omega_+ = (\Omega_c + \Omega_r)/2$, which appears in the equations for the trajectories in Cartesian coordinates[28]

$$u = x + iy = c_+e^{-i\Omega_+t} + c_-e^{-i\Omega_-t}, \tag{A7}$$

where $c_\pm$ are constants of motion that, without loss of generality, can be assumed to be real. However, from Eq. (A7), one can derive

$$r^2 = |u|^2 = c_+^2 + c_-^2 + c_+c_-[e^{i(\Omega_+-\Omega_-)t} + e^{-i(\Omega_+-\Omega_-)t}], \tag{A8}$$

so that r indeed oscillates at $\Omega_r = \Omega_+ - \Omega_-$.

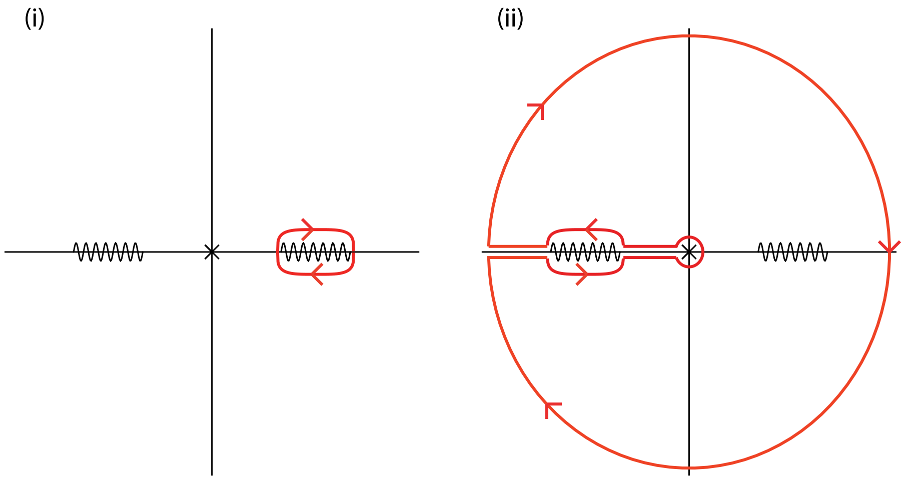

FIG. 2. Contours of integration used to evaluate the action integral for the Penning trap. The original contour, shown in (i), goes clockwise around the right-hand branch cut between the two turning points. This contour (i) can be deformed to the contour shown in (ii). The deformed contour shown in (ii) goes counterclockwise around the pole at $r=0$, counterclockwise around the left-hand branch cut, and clockwise at infinity.

APPENDIX B: FLUX ENCLOSED IN GENERALIZED COORDINATES

Equation (33), the equation for the flux enclosed by one period of motion, was derived under the assumption that two Cartesian coordinates are ignorable. Here, we generalize Eq. (33) for any set of generalized coordinates. Let $\mathbf{x}$ refer to the position vector of the particle and $\mathbf{v}$ be the velocity. Introduce a set of generalized coordinates Q^i so that $\mathbf{x}$ is a function of Q^i: $\mathbf{x}=\mathbf{x}(Q^1,Q^2,Q^3)$. It follows that

$$d\mathbf{x}=\frac{\partial \mathbf{x}}{\partial Q^i}dQ^i, \quad \mathbf{v}=\frac{d\mathbf{x}}{dt}=\frac{\partial \mathbf{x}}{\partial Q^j}\dot{Q}^j, \tag{B1}$$

where Einstein summation convention is used. We rewrite the Lagrangian for a charged particle in a magnetic field as a function of Q^i and $\dot{Q}^i$

$$L=\frac{m}{2}\mathbf{v}^2+q\mathbf{v}\cdot\mathbf{A}-qV \tag{B2}$$

$$=\frac{m}{2}\dot{Q}^i\frac{\partial \mathbf{x}}{\partial Q^i}\cdot\frac{\partial \mathbf{x}}{\partial Q^j}\dot{Q}^j+q\dot{Q}^j\frac{\partial x^i}{\partial Q^j}A_i-qV. \tag{B3}$$

The kinetic energy is typically re-expressed by defining the metric tensor g_{ij} as

$$g_{ij}=\frac{\partial \mathbf{x}}{\partial Q^i}\cdot\frac{\partial \mathbf{x}}{\partial Q^j}. \tag{B4}$$

The metric tensor relates infinitesimal displacements in the generalized coordinates, dQ^j, to the infinitesimal change in length ds

$$ds^2=d\mathbf{x}\cdot d\mathbf{x}=dQ^i\frac{\partial \mathbf{x}}{\partial Q^i}\cdot\frac{\partial \mathbf{x}}{\partial Q^j}dQ^j=dQ^ig_{ij}dQ^j. \tag{B5}$$

We write the Lagrangian as

$$L=\frac{m}{2}\dot{Q}^i\dot{Q}^jg_{ij}+q\dot{Q}^j\frac{\partial x^i}{\partial Q^j}A_i-qV, \tag{B6}$$

and the canonical momentum associated with each generalized coordinate is

$$P_i=\frac{\partial L}{\partial \dot{Q}^i}=m\dot{Q}^jg_{ij}+q\frac{\partial x^j}{\partial Q^i}A_j. \tag{B7}$$

We now split the evolution of the generalized coordinates into drift and oscillatory parts

$$\dot{Q}^i=\frac{\Delta Q^i}{\Delta t}+\dot{Q}'^i, \tag{B8}$$

where the first term is the drift velocity of the generalized coordinate and the second term is the difference between $\dot{Q}^i$ and the drift. The velocity then splits into two terms

$$\mathbf{v}=\dot{Q}^j\frac{\partial \mathbf{x}}{\partial Q^j}=\frac{\Delta Q^j}{\Delta t}\frac{\partial \mathbf{x}}{\partial Q^j}+\dot{Q}'^j\frac{\partial \mathbf{x}}{\partial Q^j}, \tag{B9}$$

which again can be identified as drift and oscillatory components.

Using Eq. (B9) in Eq. (30), we find

$$\begin{aligned}\frac{\partial J}{\partial q}&=-\int_{t_0}^{t_0+\Delta t}[-\mathbf{v}\cdot\mathbf{A}+V]dt\\&=\int_{t_0}^{t_0+\Delta t}\left[\left(\dot{Q}'^i\frac{\partial \mathbf{x}}{\partial Q^i}+\frac{\Delta Q^i}{\Delta t}\frac{\partial \mathbf{x}}{\partial Q^i}\right)\cdot\mathbf{A}-V\right]dt\\&=\Phi+\int_{t_0}^{t_0+\Delta t}\left[\frac{\Delta Q^i}{\Delta t}\frac{\partial \mathbf{x}}{\partial Q^i}\cdot\mathbf{A}-V\right]dt.\end{aligned} \tag{B10}$$

We then use Eq. (B7)

$$\begin{aligned}\frac{\partial J}{\partial q}&=\Phi+\int_{t_0}^{t_0+\Delta t}\left[\frac{1}{q}\frac{\Delta Q^i}{\Delta t}\left[P_i-m\dot{Q}^jg_{ji}\right]-V\right]dt\\&=\Phi+\frac{1}{q}\Delta Q^iP_i-\frac{m}{q}\oint\frac{\Delta Q^i}{\Delta t}g_{ji}dQ^j\\&\quad-\int_{t_0}^{t_0+\Delta t}Vdt,\end{aligned} \tag{B11}$$

which generalizes Eq. (33).

In certain instances, the third term in Eq. (B11) may be simplified. In Cartesian coordinates, for instance, the metric tensor is constant, and Eq. (B11) reduces to Eq. (33). Also, if the net displacement ΔQ^i is such that the approximation

$$\Delta\mathbf{x}=\int d\mathbf{x}=\int\frac{\partial \mathbf{x}}{\partial Q^i}dQ^i\approx\frac{\partial \mathbf{x}}{\partial Q^i}\Delta Q^i, \tag{B12}$$

is valid, then by using the definition of the metric given by Eq. (B4), we find

$$\frac{m}{q}\int_{t_0}^{t_0+\Delta t}\frac{\Delta Q^i}{\Delta t}\dot{Q}^j g_{ji}dt = \frac{m}{q}\int_{t_0}^{t_0+\Delta t}\frac{\Delta Q^i}{\Delta t}\frac{\partial \mathbf{x}}{\partial Q^i}\cdot\frac{\partial \mathbf{x}}{\partial Q^j}\dot{Q}^j dt$$
$$\approx \frac{m}{q}\int_{t_0}^{t_0+\Delta t}\left[\frac{\Delta \mathbf{x}}{\Delta t}\cdot\mathbf{v}\right]dt$$
$$= \frac{m}{q}\mathbf{v}_d\cdot\Delta\mathbf{x}, \tag{B13}$$

so that Eq. (B11) again reduces to Eq. (33). However, if Eq. (B12) is not a good approximation, then the integral in Eq. (B11) must be evaluated.

The Penning trap offers an interesting example where the integrals can be evaluated in closed form and the decomposition of flux into drift and gyro-components is clear. We begin with Eq. (B10). We can neglect the potential term in the Hamiltonian of Eq. (20) because it does not contain q and thus does not contribute to $\partial J/\partial q$. Furthermore, while there is drift motion in the z-direction, it does not contribute to Eq. (B10) because $\mathbf{x} = r\hat{r} + z\hat{z}$, so $\partial\mathbf{x}/\partial z = \hat{z}$, but $\hat{z}\cdot\mathbf{A} = 0$. Equation (B10) becomes

$$\frac{\partial J}{\partial q} = \Phi + \frac{\Delta\theta}{\Delta t}\int_{t_0}^{t_0+\Delta t}\frac{\partial\mathbf{x}}{\partial\theta}\cdot\mathbf{A}dt. \tag{B14}$$

We then have $\partial\hat{r}/\partial\theta = \hat{\theta}$, so $\partial\mathbf{x}/\partial\theta = r\hat{\theta}$. Then

$$\frac{\partial J}{\partial q} = \Phi + \frac{\Delta\theta}{\Delta t}\int_{t_0}^{t_0+\Delta t} rA_\theta dt = \Phi + \frac{\Delta\theta}{\Delta t}\frac{1}{2}B_0\int_{t_0}^{t_0+\Delta t} r^2 dt$$
$$= \Phi + \Delta\theta\frac{1}{2}B_0\langle r^2\rangle. \tag{B15}$$

The $\Delta\theta$ term is the flux enclosed by a sector of width $\Delta\theta$ and radius squared of $\langle r^2\rangle$. Over the course of a magnetron orbit, it would sum up to a flux of $\pi B_0\langle r^2\rangle$, the flux enclosed by the guiding center (e.g., magnetron) motion. Using the following identities:

$$\frac{\partial\Omega_c}{\partial q} = \frac{1}{q}\Omega_c, \quad \frac{\partial\Omega_r}{\partial q} = \frac{1}{q}\frac{\Omega_c^2}{\Omega_r}, \quad \frac{\partial\Omega_-}{\partial q} = -\frac{1}{q}\frac{\Omega_c\Omega_-}{\Omega_r}, \tag{B16}$$

one can show that differentiation of the action integral, Eq. (21), with respect to q gives

$$\frac{\partial J}{\partial q} = -\frac{1}{q}\left[2\pi\frac{\Omega_c\Omega_-}{\Omega_r^2}P_\theta + \frac{\Omega_c^2}{\Omega_r^2}J\right]. \tag{B17}$$

Then, substituting Eqs. (B17) and (27), the formula derived for $\langle r^2\rangle$, into Eq. (B15) and solving for Φ, we obtain

$$\Phi = -\frac{1}{q}\frac{\Omega_c}{\Omega_r}J. \tag{B18}$$

To verify this formula, we have run numerical simulations of a particle in a Penning trap in the particle's drift frame, which rotates with angular frequency Ω_-. In transforming from the lab frame to the rotating frame, we have added the Coriolis and centrifugal forces as well as the electric field $\mathbf{E} = \Omega_- B_0 r\hat{\theta}$ to the equations of motion. Using the particle's drift-frame trajectory to compute the magnetic flux enclosed by the orbit gives near perfect agreement with Eq. (B18).

APPENDIX C: GAUGE TRANSFORMATIONS

We show here that Eq. (33) is gauge invariant. This is expected, since the flux Φ arises from integrating $\mathbf{A}$ over the oscillatory (closed) component of the trajectory and so is unaltered if $\mathbf{A}$ is changed by the gradient of a scalar. Let primed variables represent the gauge-transformed version of the original variable, i.e., $\mathbf{A}' = \mathbf{A} + \nabla f$ and $V' = V - \partial f/\partial t$. We proceed using Cartesian coordinates; since the final result is independent of coordinate systems, the proof is general. We have $P_i' = P_i + q\partial f/\partial x_i$ and

$$H'(\mathbf{x},\mathbf{P}',q) = H(\mathbf{x},\mathbf{P}' - q\nabla f, q) - q\partial f/\partial t. \tag{C1}$$

We then take a partial derivative of H' with respect to q holding $\mathbf{x}$ and P' constant: Eq. (28), we have

$$\left.\frac{\partial H'}{\partial q}\right|_{\mathbf{P}',\mathbf{x}} = \frac{\partial}{\partial q}\left[H\left(\mathbf{x},\mathbf{P}' - q\nabla f, q\right) - q\frac{\partial f}{\partial t}\right]_{\mathbf{P}',\mathbf{x}}, \tag{C2}$$

$$= \frac{\partial H}{\partial q} + \frac{\partial H}{\partial\mathbf{P}}\cdot(-\nabla f) - \frac{\partial f}{\partial t}, \tag{C3}$$

$$= \frac{\partial H}{\partial q} - \mathbf{v}\cdot\nabla f - \frac{\partial f}{\partial t} = \frac{\partial H}{\partial q} - \frac{df}{dt}. \tag{C4}$$

Turning to Eq. (4) and using Eq. (C4), we have

$$\frac{\partial J'}{\partial q} = -\int_{t_0}^{t_0+\Delta t}\frac{\partial H'}{\partial q}dt = \frac{\partial J}{\partial q} + \Delta f, \tag{C5}$$

where Δf is the total change in f over one period of motion. Δf also appears on the right-hand side of Eq. (33). Going back to Eq. (30), we have

$$\int\mathbf{A}'\cdot d\mathbf{l} - \int V'dt = \int\mathbf{A}\cdot d\mathbf{l} - \int Vdt + \int\left[\nabla f\cdot d\mathbf{l} + \frac{\partial f}{\partial t}dt\right]$$
$$= \int\mathbf{A}\cdot d\mathbf{l} - \int Vdt + \Delta f. \tag{C6}$$

This shows that the right-hand side of Eq. (30) transforms in the same fashion as the left-hand side, so that Eq. (33) is invariant.

Note that one could choose a "pathological" gauge in which the phase-space trajectory projected onto the xP_x plane is not closed. For instance, adding the gauge $f(x,y) = kxy^2$, where k is some constant of proportionality, produces the gauge-transformed x canonical momentum $P_x' = P_x + q\partial f/\partial x = P_x + qky^2$, which grows quadratically in time on average whenever there is a drift in the y direction. The xP_x projection of the orbit is therefore no longer closed, not even approximately. The trajectories in physical space are, of course, independent of gauge, but the action-integral formalism fails under particular gauge transformations. By analogy, a magnetic field may exhibit a certain symmetry, and one would expect to find a conserved momentum associated with that symmetry, but one can choose a gauge that does not share the same symmetry as the magnetic field so that the momentum in the symmetry direction is not conserved. As the adiabatic invariance of J is essentially due to an averaged symmetry of the system with respect to the phase of the motion, one might wish to choose gauges that observe this symmetry in order to employ the action-integral formalism.

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