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An expectation value formulation of the perturbed Kepler problem

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A classical formulation of the nonrelativistic Kepler problem in terms of expectation values of powers of the radial coordinate r is presented. Perturbations to this problem arising from relativistic corrections to the kinetic and potential energies, multipole moments of the central potential, other confocal orbitals, etc. can be written in terms of powers of r and thus be accounted for through these expectation values in a simple and pedagogically transparent way. Macroscopic and microscopic examples are treated as special cases of this common formulation.

I. INTRODUCTION

The advance of the perihelion of the planet Mercury[1–5] and the term structure of atomic spectral lines[6–8] are subjects often included in a first course in elementary modern physics. They are, however, usually presented using quite different mathematical formalisms, and relationships between them (if included) are reserved for a discussion of the "correspondence limit" of quantum theories.[9–11] Much of the difference in the presentation arises not from quantum mechanical effects in the microscopic case, but from a nonessential heuristic tendency to describe macroscopic systems by instantaneous quantities and microscopic systems by time-averaged expectation values.

Undergraduate students typically have a knowledge of the Newton's law formulation of mechanics and the technical use of quantum mechanical operations, but the connection between the two through Hamilton–Jacobi methods is not made clear until graduate study. For nearly periodic systems it is possible to present both macroscopic and microscopic systems in a unified and pedagogically transparent exposition using orbit-averaged expectation values.

It will be shown that expectation values for powers of the radial coordinate in the Kepler problem can be exactly described by a general algebraic formula. This result will be applied to compute perturbations to the problem arising from relativistic corrections to the kinetic and potential energies, from multipole moments of a general central potential, and from other confocal orbitals.

II. EXPECTATION VALUE FORMULATION OF THE CLASSICAL NONRELATIVISTIC KEPLER PROBLEM

Gravitational systems in a nonrelativistic attractive $1/r$ potential are usually cast in terms of Kepler's three laws,[4]

$$1/r = [1 + (1 - b^2/a^2)^{1/2} \cos\theta]a/b^2, \tag{1}$$

$$r^2 \frac{d\theta}{dt} = \frac{2\pi ab}{\tau}, \tag{2}$$

$$\tau = 2\pi a^{3/2}(m/k)^{1/2}, \tag{3}$$

where r and θ are the standard two-dimensional polar coordinates, a and b are the semimajor and semiminor axes of the elliptic orbit, τ is the period of the orbit, $-k$ is the potential energy at unit radius, and m is the orbiting mass. (In standard symbols, $k = GMm$ for gravitation and $k = -Qq/4\pi\epsilon_0$ for electrostatics.) Since the standard reduction to center of momentum and relative coordinates separates only in the lowest nonrelativistic approximation, an infinitely massive central attractor will be assumed throughout. This orbital locus approach is not essential to the classical problem, which can be very concisely described in terms of expectation values in closer analogy with the corresponding quantum mechanical problem.

The orbital time average of integer powers of the radial coordinate can be converted to an angular average through Eq. (2),

$$\langle r^s \rangle = \frac{1}{\tau}\int_0^\tau dt\, r^s = \frac{1}{2\pi ab}\int_0^{2\pi} d\theta\, r^{s+2} \tag{4}$$

and can be further reduced, using Eq. (1), to

$$\langle r^s \rangle = \frac{b^{2s+3}}{\pi a^{s+3}}\int_0^\pi d\theta \left[1 + \left(1 - \frac{b^2}{a^2}\right)^{1/2}\cos\theta\right]^{-s-2}. \tag{5}$$

The basis for the simplicity of the formulation presented here rests on recognizing that Eq. (5) can be integrated exactly, using standard tabulated forms[12,13] to obtain a general algebraic expression. Depending upon whether $-s-2$ is positive or negative, the trigonometric integral in Eq. (5) corresponds either to formula 3.661 – 3 or

3.661 — 4 in the integral tables of Ref. 12, where it is shown to yield the exact algebraic expression

$$\langle r^s \rangle = b^s (b/a) P_{|s+3/2|-1/2}(a/b) . \tag{6}$$

Here $P_i(x)$ is the Legendre polynomial (in an unusual physical case where $x \geqslant 1$). The index $i = |s+\frac{3}{2}| - \frac{1}{2}$ is symmetric about $s = -\frac{3}{2}$ and is constructed to yield $i = s+1$ for $s \geqslant -1$ and $i = -s-2$ for $s \leqslant -2$. The details of the contour integration by which this result can be obtained are given in Ref. 13. Equation (6) provides a convenient context for a perturbative study of small deviations from the Kepler problem, and while the integral was known to (and applied to planetary motion by) Laplace prior to 1825,[14] the application described here appears to have been overlooked until recently.[6]

We define the unperturbed potential energy as

$$V_0 = -k/r \tag{7}$$

and the nonrelativistic kinetic energy as

$$T_0 = p^2/2m. \tag{8}$$

Notice that the alternative definition $mv^2/2$ for the nonrelativistic kinetic energy is equivalent to Eq. (8) only in lowest order, and yields a different expansion when higher order corrections are included. As discussed in Sec. V, p is the quantity appropriate to the Hamiltonian formulation.

The virial theorem[4] for this system yields a total energy $E_0 = T_0 + V_0$ given by

$$E_0 = -\langle T_0 \rangle = \tfrac{1}{2}\langle V_0 \rangle = -k/2a . \tag{9}$$

Add to this the expression for the angular momentum L obtained from Eqs. (2) and (3),

$$L = b(mk/a)^{1/2} \tag{10}$$

and it is possible to use these equations to describe perturbations to the systems in very elementary terms.

III. PERTURBATIONS: ENERGY SHIFTS AND PERIHELION ADVANCE

Small deviations from a Keplerian system can often be expressed as a perturbative central potential which is given or approximated by a power law in the radial coordinate

$$\Delta E = k' r^s . \tag{11}$$

The energy of the perturbed system can be approximated by

$$E = E_0 + \langle \Delta E \rangle + \cdots , \tag{12}$$

where the average is taken over the unperturbed orbit

$$\langle \Delta E \rangle = k' \langle r^s \rangle . \tag{13}$$

In atomic systems, perturbations are usually described directly in terms of these energy shifts. The shift relative to the unperturbed energy is a useful dimensionless quantity

$$\langle \Delta E \rangle / E_0 = -(2ak'/k)\langle r^s \rangle . \tag{14}$$

The expectation value can be evaluated in terms of a and b using Eq. (6). While this is an equally valid description of the gravitational problem, historical tradition favors its exposition in terms of the apsidal advance, which pertains to the atomic problem only in the correspondence limit. Since the apsidal advance is determined through observations on a time scale during which all planets involved have undergone many orbital periods, instantaneous orbit positions need not be considered and a formulation in terms of time-averaged position probability densities and expectation values is quite appropriate to both the microscopic and macroscopic examples. The classical advance of the perihelion corresponding to the energy given in Eq. (12) can be deduced quite simply. Using the Hamilton–Jacobi angle-action variable formulation of perturbation theory, the precessional angular velocity $\langle \omega \rangle$ is given by [see Eq. (11.42) of Ref. 4]

$$\langle \omega \rangle = \left(\frac{\partial \langle \Delta E \rangle}{\partial L} \right)_{E_0 = \text{const}} . \tag{15}$$

Since E_0 corresponds to $1/a$ [Eq. (9)] and L corresponds at constant E_0 to b [Eq. (10)], the precession (in rad/rev) can be written [using Eqs. (3), (9), (10), (13), and (15)] as

$$\langle \omega \rangle \tau = 2\pi \frac{a^2 k'}{k} \left(\frac{\partial \langle r^s \rangle}{\partial b} \right)_{a = \text{const}} . \tag{16}$$

This derivative can be evaluated formally from Eq. (6) using the differential properties of the Legendre polynomial

$$\left(\frac{\partial \langle r^s \rangle}{\partial b} \right)_a = \frac{a^{s-1}}{x^s} \left((s+1) P_i(x) + \frac{ix}{1-x^2} [x P_i(x) - P_{i-1}(x)] \right), \tag{17}$$

where $x = a/b$ and $i = |s+\frac{3}{2}| - \frac{1}{2}$. Equation (16) can be evaluated for specific values of a and b either by numerical computation of the Legendre polynomials in Eq. (17), or by functional evaluation and differentiation of Eq. (6).

IV. EXPLICIT VALUES FOR a AND b

The formulation presented here is independent of whether a and b are interpreted as semiaxes of a physical ellipse or as discrete quantum mechanical eigenvalues. In the gravitational case the definition of a and b from an observable ellipse is clear, but in the quantum mechanical case a and b can also be given a precise and rigorous meaning. To see this, we begin by considering the semiclassical approximation, but we will show that the representation of a and b can be generalized to be fully quantum mechanical. In the Einstein–Keller–Brillouin semiclassical formulation,[7] the semimajor and semiminor axes are given by

$$a = a_0 n^2 \tag{18}$$

and

$$b = a_0 n (l + \tfrac{1}{2}) , \tag{19}$$

where a_0 is the Bohr radius (5.29 nm) and n and l are the principal and orbital angular momentum quantum numbers. Semiclassical values for $\langle r^s \rangle$ can be obtained through the substitution of Eqs. (18) and (19) into Eq. (6). For $s = 0$, -1, and -2 the semiclassical and quantum mechanical results are identical and Eq. (6) is correctly specified quantum mechanically by Eqs. (18) and (19). Furthermore, the corresponding quantum mechanical expressions can be formed from the semiclassical results through a simply structured substitution for b^j when $|j| > 1$. In this substitution, the expectation value of L raised to higher powers is not obtained by successive multiplication by $(l + \frac{1}{2})$, but from formulas prescribed in Eqs. (19) and (18) of Ref. 6. For example, the replacement for b^3 is

$$b^3 \rightarrow (a_0 n)^3 l (l + \tfrac{1}{2})(l+1). \tag{20}$$

Table I. Data used in examples. For conversions from rad/rev to arcsec/century, the period of Mercury is 0.2409 yr.

System	a	a/b	k/mc^2a
Hydrogen 1s	$1\,a_0$	2	$1/137^2 = 5.33\times10^{-5}$
Hydrogen 2s	$4\,a_0$	$\frac{4}{3}$	1.33×10^{-5}
Planet Mercury	0.387 AU	1.022	2.55×10^{-8}

Thus if powers of b are interpreted to represent the appropriate values, Eq. (14) represents the graviational and both the semiclassical and quantum mechanical atomic problems as an explicit function of a and b. Equation (16) shifts the power of b and should be considered only in the correspondence limit. For examples that will be treated below, values for a and b and the dimensionless strength parameter k/mc^2a are given in Table I. Since the perturbation is relatively small for the planetary case the unperturbed values of a and b are approximated by their physical values.

V. RELATIVISTIC CORRECTIONS TO THE KINETIC ENERGY

The first correction we shall consider is the relativistic kinetic energy, which can be written as

$$T=[(mc^2)^2+(pc)^2]^{1/2}-mc^2. \tag{21}$$

This can be binomial expanded to yield

$$T=mc^2\left[1+\tfrac{1}{2}(p/mc)^2-\tfrac{1}{8}(p/mc)^4+\cdots\right]-mc^2 \tag{22}$$

and can be simplified and rewritten using Eq. (8):

$$T=T_0-T_0^2/2mc^2+\cdots. \tag{23}$$

Notice that Eq. (21) could alternatively have been written in terms of the velocity and expanded to obtain a series in powers of $mv^2/2$ with coefficients different from those in Eq. (22). The two expansions are equivalent if the relativistic relationship between momentum and velocity is inserted, but the Hamiltonian formulation is based upon partial derivatives with respect to momentum (with other quantities held constant), not velocity, and these are not relativistically equivalent. Thus the momentum formulation of Eq. (22) provides the more convenient expansion.

The perturbation defined in Eq. (12) for this case is given by

$$\langle\Delta E\rangle=\langle T\rangle-\langle T_0\rangle=-\langle T_0^2\rangle/2mc^2. \tag{24}$$

This can be written in terms of known quantities using $E_0=T_0+E_0$ by considering

$$\langle T_0^2\rangle=\langle(E_0-V_0)^2\rangle=E_0^2-2E_0\langle V_0\rangle+\langle V_0^2\rangle. \tag{25}$$

Using Eqs. (9) and (25), Eq. (24) becomes

$$\langle\Delta E\rangle=-(1/2mc^2)\left(\langle V_0^2\rangle-\tfrac{3}{4}\langle V_0\rangle^2\right)+\cdots \tag{26}$$

and using Eq. (6), the correction to the energy is written as

$$\langle\Delta E\rangle=-(k^2/2mc^2)(1/ab-3/4a^2). \tag{27}$$

The relative splitting is

$$\langle\Delta E\rangle/E_0=(k/mc^2a)(a/b-\tfrac{3}{4}) \tag{28}$$

and the perihelion advance is

$$\langle\omega\rangle\tau=\pi(k/mc^2a)(a/b)^2. \tag{29}$$

Examples can be computed using the data in Table I. For the 1s electron in hydrogen Eq. (28) yields 6.66×10^{-5} and Eq. (29) yields 6.69×10^{-4} rad/rev. For the planet Mercury Eq. (28) yields 6.94×10^{-9} and Eq. (29) yields 8.37×10^{-8} rad/rev (7.2 arcsec/century). These equations thus describe both Sommerfeld's fine structure corrections to the Bohr atom and the special relativistic mass contribution to the advance of the perihelion of Mercury.

VI. RELATIVISTIC CORRECTIONS TO THE POTENTIAL ENERGY

A. General relativity

When general relativistic methods are applied to the gravitational problem, the Schwarzschild solution of the Einstein field equations corresponds to a perturbation of form[4]

$$\langle\Delta E\rangle=-[kL^2/(mc)^2]\langle r^{-3}\rangle. \tag{30}$$

The quantity L^2 in the numerator of Eq. (30) corresponds numerically to the orbital angular momentum, but as Goldstein has cautioned (Ref. 4, p. 512), in this context L^2 is a constant and not a canonical momentum and is not acted upon by the derivative in Eq. (15). The perturbation potential is a function of dynamical variables only through $\langle r^s\rangle$ as given in Eq. (16). In the general relativity case, the relative energy separation from Eqs. (6), (12), and (30) is

$$\langle\Delta E\rangle/E_0=2(k/mc^2a)(a/b) \tag{31}$$

and the perihelion advance from Eqs. (6) and (16) is

$$\langle\omega\rangle\tau=6\pi(k/mc^2a)(a/b)^2. \tag{32}$$

For the planet Mercury this gives a precession of its perihelion of 43 arcsec/century. This is in agreement with observation, but is six times the amount predicted by special relativistic corrections to the kinetic energy in Sec. V. An additional special relativistic correction has been proposed[1] that invokes the principle of equivalence to obtain a velocity-dependent gravitational force. This method reduces the discrepancy between special relativity and observation to a factor of 2 and the development can be carried through by the methods discussed here. Factors of 2 between results computed by special and general relativity often occur and have recently been discussed by Strandberg.[5] There are, however, subtleties associated with this velocity-dependent potential that make it less suitable as a pedagogic example.

B. Spin-orbit coupling

For the electromagnetic interactions, the relativistic corrections to the potential energy involve magnetic interactions. Through a standard development (Ref. 15 and the citations therein) using the Biot–Savart Law, the anomalous magnetic moment of the electron, and the Thomas precession, this leads to a further correction of the form (with the effect of the anomolous moment of the electron

incorporated into the constant k)

$$\langle \Delta E \rangle = [k \langle \mathbf{L}\cdot\mathbf{S} \rangle / 2(mc)^2] \langle r^{-3} \rangle, \tag{33}$$

where $\langle \mathbf{L}\cdot\mathbf{S} \rangle$ involves quantum mechanical expectation values for the orbital and spin angular momentum operators. It is worth noting the similarities between Eq. (33) from spin orbit and Eq. (30) from general relativity, observing that both L^2 and $\langle \mathbf{L}\cdot\mathbf{S} \rangle$ have dimensions of angular momentum squared.

In the case of the spin-orbit energy, the potential differs from other examples given here, since, unlike orbital angular momentum, electron spin cannot be described in terms of spatial coordinates or ellipse axes. Thus while the quantization conditions in $\langle r^s \rangle$ can remain implicit in a and b, the quantity $\langle \mathbf{L}\cdot\mathbf{S} \rangle$ introduces a partial quantization. If we consider the difference between two spin-$\frac{1}{2}$ states that differ only in total angular momentum (in units of Planck's constant $\hbar$) $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$, Eq. (33) becomes (using the vector model of angular momentum)

$$\frac{\langle \Delta E(l + 1/2) - \Delta E(l - 1/2) \rangle}{E_0} = -\frac{\hbar^2 (l + 1/2)}{(mc)^2} \frac{a}{b^3}. \tag{34}$$

The difference in the classical perihelion advance for these two orbitals corresponds to

$$\Delta \langle \omega \rangle \tau = -\{[6\pi \hbar^2 (l + 1/2)]/(mc)^2\}(a^2/b^4). \tag{35}$$

Equations (34) and (35) can be further simplified by substituting $(\hbar/mc)^2 = ka_0/mc^2$. The fine structure of the $2p$ levels in hydrogen can be computed using Table I and Eqs. (18) and (20). This yields 1.33×10^{-5} for Eq. (34) and 2.97×10^{-4} rad/rev for Eq. (35).

When the spin orbit and relativistic kinetic energy terms for the hydrogen atom are combined, the resulting expression can be reduced to a form identical to the relativistic kinetic energy alone, Eq. (27), except that the orbital angular momentum quantum number l is replaced by the total angular momentum quantum number j. This corresponds to the result of Dirac theory to order $(E_0/mc^2)^2$.

VII. CORRECTIONS FOR HIGHER ORDER MULTIPOLE MOMENTS

In the atomic case, the core electrons can acquire induced dipole and quadrupole polarization moments. Denoting the dipole and quadrupole polarizabilities by α_d and α_q, the perturbation is[6]

$$\langle \Delta E \rangle = -\tfrac{1}{2} k [\alpha_d \langle r^{-4} \rangle + \alpha_q \langle r^{-6} \rangle], \tag{36}$$

which, using Eq. (6), becomes

$$\langle \Delta E \rangle = -\frac{1}{2} k \left[\alpha_d \left(3 - \frac{b^2}{a^2} \right) \frac{a}{2b^5} + \alpha_q \left(35 - 30 \frac{b^2}{a^2} + 3 \frac{b^4}{a^4} \right) \frac{a^3}{8b^9} \right]. \tag{37}$$

Perturbations can also arise due to permanent quadrupole moments (solar oblateness, nuclear hyperfine structure, etc.) of the central potential. For an orbit in the equatorial plane of the central mass M, this potential is of the form

$$\langle \Delta E \rangle = \tfrac{1}{2} kQ \langle r^{-3} \rangle = kQ/2b^3, \tag{38}$$

where Q is the quadrupole moment in units of the central charge or mass.

VIII. CORRECTIONS FOR OTHER PLANETS OR CONFOCAL ORBITALS

Perturbations on a planetary orbit due to other planets can also be described by this formalism. Since these effects are usually measured over hundreds of years, the planets involved have completed many orbits, and the time average approach is appropriate. The situation is very similar to the quantum mechanical case, in which instantaneous positions can be replaced by time-averaged position probability densities. As a simple pedagogic model, a procedure first utilized by Gauss[16] is followed in which each perturbing planet is here replaced by a uniform circular ring having the same mass as the planet and a radius corresponding to the appropriate moment of the planet's orbit about the sun (cf. also Ref. 3). The potential at any point in space due to a ring of charge or mass is given by[17]

$$V(r,\theta) = k \sum_{j=0}^{\infty} \frac{r_<^j}{r_>^{j+1}} P_j(\cos\alpha) P_j(\cos\theta). \tag{39}$$

where α and θ are the angles between the axis of the ring and the source and field points. Within the plane of the ring $\alpha = \theta = \pi/2$. We denote the mass and radial coordinate of the ith perturbing planet by M_i and R_i and the mass of the sun by M_s.[18] For a perturbing planet interior to the orbit

Table II. Precession of the perihelion of Mercury (in arcsec/century) due to perturbations of the other planets. Calculations using the simple ring model of Sec. VIII are compared with the detailed calculations of Clemence,[19] who compares the observed perihelion advance of 5599.74 arcsec/century with calculated contributions of 5025.65 from equinox precession of the Earth, 531.50 from perturbations by other planets, and 43.03 from general relativity.

Perturbing planet	Ring model one term	Ring model three terms	Ring model 50 terms	Clemence[19]
Venus	148.298	267.359	293.237	277.856
Earth and Moon	69.715	94.696	96.018	90.038
Mars	2.130	2.434	2.437	2.536
Jupiter	155.948	157.646	157.646	153.584
Saturn	7.586	7.611	7.611	7.302
Uranus	0.143	0.143	0.143	0.141
Neptune	0.044	0.044	0.044	0.042
Total	383.863	529.933	557.136	531.499

considered, the potential is given by the infinite series

$$\langle \Delta E \rangle = -(kM_i/M_s)[\langle r^{-1}\rangle + (\tfrac{1}{2})^2\langle R_i^2\rangle\langle r^{-3}\rangle + (1*3/2*4)^2\langle R_i^4\rangle\langle r^{-5}\rangle + \cdots]. \quad (40)$$

This series for the interior planets corresponds to a multipole expansion and is a generalization of the quadrupole moment given in Eq. (38). The monopole moment in Eq. (40) could be incorporated into the unperturbed solution to improve the values of a and b used in higher moments. For a perturbing planet outside the orbit considered, the potential is given by the infinite series

$$\langle \Delta E \rangle = -(kM_i/M_s)[\langle R_i^{-1}\rangle + (\tfrac{1}{2})^2\langle R_i^{-3}\rangle\langle r^2\rangle + (1*3/2*4)^2\langle R_i^{-5}\rangle\langle r^4\rangle + \cdots]. \quad (41)$$

We have utilized Eq. (41) to make an illustrative determination of the perturbations on the orbit of the planet Mercury due to all the other planets. The advance of the perihelion corresponding to Eqs. (41) and (16) is, to the lowest order,

$$\langle \omega \rangle \tau = (3\pi/2)(M_i/M_s)(a^2 b/B_i), \quad (42)$$

where B_i is the semiminor axis of the orbit of the ith perturbing planet. Additional terms in Eq. (41) were computed using a computer algorithm for generating Legendre polynomials in Eqs. (6) and (17). Table II compares the predictions of the expansion in Eqs. (16) and (41) with each other and with the more sophisticated calculations of Clemence,[19] including the first term [Eq. (42)], the first three terms and the first 50 terms. Agreement is quite good for planets beyond the Earth, irrespective of the number of terms included. For corrections due to Venus and the Earth the agreement first improves, but then worsens. Inclusion of terms beyond the first correction of Eq. (42) is not quantitatively justified here since higher order contributions to Eq. (12) will mix perturbation and multipolarity orders. However, even if only the lowest correction of Eq. (42) is included, this approach does provide a useful pedagogic device for the exposition of these perturbations. As another application, a variation of this approach could be used to model inner electron screening in optical atomic spectra and outer electron screening in x-ray spectra.

IX. DISCUSSION

The use of semiclassical Bohr orbits as a pedagogic introduction to atomic physics is often criticized as involving an archaic and unnecessary step in the formulation of modern quantum theory. However, similar arguments could be made concerning the use of forces and instantaneous coordinates as the obligatory introduction to the study of macroscopic mechanics. Through the use of expectation values and energy perturbation expansions, real analogies between macroscopic and microscopic systems emerge which are independent of quantization considerations and which provide a unity and economy of presentation.

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