Use of the Einstein–Brillouin–Keller action quantization

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The Einstein–Brillouin–Keller semiclassical quantization and the topological Maslov index are used to deduce the correct quantum mechanical values for the energy of a one-electron atom (both nonrelativistically and relativistically) and a three-dimensional harmonic oscillator. The development is concise, transparent, and involves only elementary integral calculus and provides a conceptual and intuitive introduction to the quantum nature of the atomic and molecular structure of matter.
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I. INTRODUCTION

A simple semiclassical means for obtaining correct quantum mechanics results without invoking the full mathematics of the Schrödinger equation is provided by the Einstein–Brillouin–Keller (EBK) action quantization.[1–3] Although this approach is a well-known tool in contemporary atomic and molecular theory, its usefulness and pedagogical value has been largely overlooked in elementary textbooks. Unfortunately, textbooks tend to perpetuate and then disparage the flawed and archaic Bohr–Sommerfeld–Wilson quantization,[4–6] which (as was recognized shortly after its introduction)[1] fails to properly account for caustic phase jumps at the classical turning points.

The EBK quantization approach[1–3] involves a path integral over the phase space of each coordinate q_i and its conjugate momentum p_i, given by

$$\left(n_i+\frac{\mu_i}{4}\right)\hbar=\frac{1}{2\pi}\oint dq_i\,p_i, \tag{1}$$

where $n_i=0,1,2,\cdots$, μ_i is the Maslov index,[7] which is the total phase loss during one period in units of $\pi/2$, and $\hbar$ has its usual meaning. For example, each classical turning point (or caustic) and each reflection contributes one unit to μ_i.

EBK quantization has been applied to one-dimensional examples,[8] quantum defect formulations,[9] the one-dimensional harmonic oscillator,[10] atoms in strong magnetic fields,[11] and many other interesting systems. Our purpose here is to review the application of the method and show that it also can be used to obtain the correct quantum mechanical energy values for both the one-electron problem and the three-dimensional isotropic harmonic oscillator.

II. SPHERICAL POLAR COORDINATE FORMULATION

We will use the usual three-dimensional spherical polar coordinates r, ϑ, and φ, where ϑ is the azimuthal angle specifying the tilt of the orbital plane relative to an arbitrarily chosen z axis. If the radial coordinate has distances of closest approach and greatest recession denoted by r_1 and r_2, and the normal to the plane of the orbit makes an angle Θ with the z axis, then the ranges of the coordinates over the orbital motion are given by

$$r_1\leqslant r\leqslant r_2, \tag{2a}$$

$$\pi/2-\Theta\leqslant\vartheta\leqslant\pi/2+\Theta, \tag{2b}$$

$$0\leqslant\varphi\leqslant 2\pi. \tag{2c}$$

Thus r and ϑ undergo librations (oscillate between two endpoints) and φ undergoes a rotation.

The momenta associated with these three coordinates can be motivated for beginning students on the basis of conservation of energy. However, for background clarity, the generalized momenta will be obtained using the Hamilton–Jacobi formalism.[12] This formalism involves the construction of the Lagrangian in terms of the coordinates q_i and their time derivatives $\dot{q}_i$. The generalized momentum canonical to the coordinate q_i is obtained by differentiating the Lagrangian with respect to $\dot{q}_i$. The Hamiltonian is then formed by reexpressing the $\dot{q}_i$ quantities in terms of the generalized momenta. For this case, the Hamiltonian is given by

$$H=\frac{1}{2m}\left(p_r^2+\frac{p_\vartheta^2}{r^2}+\frac{p_\varphi^2}{r^2\sin^2\vartheta}\right)+V(r). \tag{3}$$

Because the potential does not involve angular coordinates, the ϑ and φ momenta can be separated

$$p_\varphi^2=\text{constant},\quad p_\vartheta^2+\frac{p_\varphi^2}{\sin^2\vartheta}=\text{constant}. \tag{4}$$

We denote the first constant as L_z^2, the second constant as L^2, and the Hamiltonian energy as E, and write

$$p_\varphi=L_z,\quad p_\vartheta=\sqrt{L^2-\frac{L_z^2}{\sin^2\vartheta}}, \tag{5}$$

and

$$p_r=\sqrt{2m[E-V(r)]-L^2/r^2}. \tag{6}$$

The phase integrals for the Kepler and isotropic harmonic oscillator problems consist of two librations (one in r and one in ϑ) and one rotation (in φ). All three integrals are known forms[8] and have been obtained by methods that have been discussed in detail.[13,12] The phase integrals are

$$\left(n_r+\frac{1}{2}\right)\hbar=\frac{1}{2\pi}\oint dr\sqrt{2m[E-V(r)]-\frac{L^2}{r^2}}, \tag{7}$$

$$\left(n_\vartheta+\frac{1}{2}\right)\hbar=\frac{1}{2\pi}\oint d\vartheta\sqrt{L^2-\frac{L_z^2}{\sin^2\vartheta}}=L-L_z, \tag{8}$$

$$n_\varphi\hbar=\frac{1}{2\pi}\oint d\varphi\,L_z=L_z. \tag{9}$$

The r quantization in Eq. (7) requires the specification of $V(r)$. The ϑ and φ quantizations of Eqs. (8) and (9) are the same for any central potential.[12] If Eqs. (8) and (9) are added, we obtain

$$\left(n_\vartheta + n_\varphi + \frac{1}{2}\right)\hbar = L. \tag{10}$$

To obtain a notation consistent with that utilized in the corresponding quantum mechanical formulation, we denote

$$\ell \equiv n_\vartheta + n_\varphi \tag{11}$$

$$m_\ell \equiv \pm n_\varphi, \tag{12}$$

where the $\pm$ indicates a counterclockwise or clockwise azimuthal integration. In this notation,

$$L = \left(\ell + \frac{1}{2}\right)\hbar \tag{13}$$

$$L_z = m_\ell \hbar. \tag{14}$$

Note that the value for $L^2/\hbar^2 = (\ell + \frac{1}{2})^2 = (\ell^2 + \ell + \frac{1}{4})$ agrees with the quantum mechanical result $\ell(\ell+1)$ for $\ell \gg 1$.

For the radial integration, a useful integral is

$$\frac{1}{2\pi} \oint \frac{dz}{z} \sqrt{Az^2 + 2Bz - C} = -\sqrt{C} + \frac{B}{\sqrt{-A}}. \tag{15}$$

The proof of this equality using contour integration (with poles at $z=0$ and $1/z=0$) is described in Ref. 12; the result will be used in the discussion that follows.

III. APPLICATIONS

A. One-electron atom or ion (nonrelativistic)

For a hydrogen atom (or a hydrogenlike ion with nuclear charge Z) the potential is

$$V(r) = -KZe^2/r. \tag{16}$$

This potential leads to the radial EBK quantization integral

$$\left(n_r + \frac{1}{2}\right)\hbar = \frac{1}{2\pi} \oint dr \sqrt{2m\left(E + \frac{KZe^2}{r}\right) - \frac{L^2}{r^2}} = \frac{1}{2\pi} \oint \frac{dr}{r} \sqrt{2mEr^2 + 2mKZe^2 r - L^2}. \tag{17}$$

Equation (17) can be evaluated using Eq. (15), with $A = 2mE$, $B = mKZe^2$, and $C = L^2$ to obtain

$$\left(n_r + \frac{1}{2}\right)\hbar = -L + KZe^2\sqrt{-\frac{m}{2E}}. \tag{18}$$

From Eq. (13), we have

$$\left(n_r + \frac{1}{2}\right)\hbar + L = (n_r + \ell + 1)\hbar, \tag{19}$$

and we define the principal quantum number n as

$$n \equiv n_r + \ell + 1 = n_r + n_\vartheta + n_\varphi + 1. \tag{20}$$

The substitutions $Ke^2 = 2R_y a_0$ and $\hbar^2/m = 2R_y a_0^2$ are convenient in converting to atomic units. In these units, the energy is given by

$$E = -R_y Z^2/n^2. \tag{21}$$

The values for E, L_z, and the correspondence limit of L^2 agree with the predictions of nonrelativistic Schrödinger theory.

B. One-electron atom or ion (relativistic)

Although there are problems[12] associated with obtaining a relativistically covariant description within the Hamiltonian approach, it is possible to incorporate relativistic momentum corrections into this formulation. For an electrostatic Coulomb potential, the relativistic energy can be written as

$$E + mc^2 = \sqrt{(pc)^2 + (mc^2)^2} - KZe^2/r. \tag{22}$$

We rewrite Eq. (22) as

$$[(E + mc^2) + KZe^2/r]^2 = (pc)^2 + (mc^2)^2, \tag{23}$$

and solve for $(pc)^2$:

$$(pc)^2 = \left(p_r^2 + \frac{L^2}{r^2}\right)c^2 = E(E + 2mc^2) + \frac{2KZe^2}{r} \times (E + mc^2) + \frac{(KZe^2)^2}{r^2}, \tag{24}$$

which can be rewritten as

$$p_r^2 = 2mE\left(1 + \frac{E}{2mc^2}\right) + \frac{2mKZe^2}{r}\left(1 + \frac{E}{mc^2}\right) - \frac{1}{r^2}[L^2 - (KZe^2/c)^2]. \tag{25}$$

Equation (25) can be expressed in terms of atomic units by noting that the fine structure constant $\alpha \equiv Ke^2/\hbar c$. Thus, the radial dependence of the relativistic form of p_r is the same as that of the nonrelativistic form, if we make the association

$$A = 2mE\left(1 + \frac{E}{2mc^2}\right) \tag{26a}$$

$$B = mKZe^2\left(1 + \frac{E}{mc^2}\right) \tag{26b}$$

$$C = [L^2 - (\alpha Z\hbar)^2]. \tag{26c}$$

The radial EBK condition becomes

$$\left(n_r + \frac{1}{2}\right)\hbar = -\sqrt{L^2 - (\alpha Z\hbar)^2} + \frac{mKZe^2(1 + E/mc^2)}{\sqrt{-2mE(1 + E/2mc^2)}}. \tag{27}$$

We use Eq. (13)

$$n - \ell - \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2}\right)^2 - (\alpha Z)^2} = \frac{\alpha Z(1 + E/mc^2)}{\sqrt{-2E/mc^2(1 + E/2mc^2)}}, \tag{28}$$

and obtain

$$(E+mc^2) = mc^2\left\{1+\frac{(\alpha Z)^2}{\left[n-\ell-\frac{1}{2}+\sqrt{\left(\ell+\frac{1}{2}\right)^2-(\alpha Z)^2}\right]^2}\right\}^{-1/2}. \quad (29)$$

Equation (29) is the relativistic equation obtained by Sommerfeld.[5] Note that if the orbital angular momentum ℓ in this semiclassical expression is replaced by the total (orbital plus spin) angular momentum j, the correct relativistic expression for the Dirac energy is obtained.

By taking differences between the Dirac energies for the two values of the total angular momentum $j=\ell+\frac{1}{2}$ and $j=\ell-\frac{1}{2}$ (corresponding to the parallel and antiparallel alignment of the spin and orbital angular momentum), the fine structure separation can be specified. This calculation can be done directly, or (for students with more mathematical facility) using a closed form series expansion[14] for Eq. (29), the first two terms of which are

$$E=-\frac{mc^2}{2}\left[\left(\frac{\alpha Z}{n}\right)^2+\left(\frac{\alpha Z}{n}\right)^4\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\right], \quad (30)$$

which can be compared with the nonrelativistic expression by noting that $R_y=mc^2\alpha^2/2$.

C. Isotropic harmonic oscillator

The potential of an isotropic harmonic oscillator is

$$V(r)=\frac{1}{2}m\omega^2r^2. \quad (31)$$

Equation (31) leads to the radial EBK quantization integral

$$\left(n_r+\frac{1}{2}\right)\hbar=\frac{1}{2\pi}\oint dr\sqrt{2mE-m^2\omega^2r^2-\frac{L^2}{r^2}} = \frac{1}{2\pi}\oint\frac{dr}{r}\sqrt{2mEr^2-m^2\omega^2r^4-L^2}. \quad (32)$$

The substitution $z=r^2$ transforms Eq. (32) to

$$\left(n_r+\frac{1}{2}\right)\hbar=\frac{1}{2}\frac{1}{2\pi}\oint\frac{dz}{z}\sqrt{2mEz-m^2\omega^2z^2-L^2}, \quad (33)$$

which is of the form of Eq. (15) with $A=-m^2\omega^2$, $B=mE$, and $C=L^2$, and yields

$$\left(n_r+\frac{1}{2}\right)\hbar=\frac{1}{2}\left[-L+\frac{E}{\omega}\right]. \quad (34)$$

We again use Eq. (13) and find

$$E=\left(2n_r+\ell+\frac{3}{2}\right)\hbar, \quad (35)$$

where the principal quantum number is defined as

$$n\equiv 2n_r+\ell=2n_r+n_\vartheta+n_\varphi. \quad (36)$$

IV. CONCLUSION

Our results provide a compact introduction to the quantum nature of matter, without the need for a knowledge of partial differential equations, infinite series, complex variables, or the other mathematical tools of quantum mechanics.

The introduction of the quantization of action also fits in well with the fundamental role played by this quantity in the principle of least action. In a recent essay,[15] Taylor suggested the use of least action methods as a more flexible and more powerful teaching approach than traditional Newtonian mechanics. It has been shown[8] that Newtonian physics can be expressed in terms of classical position probability densities by examining the ''dwell time patterns'' given by the reciprocal speed. The use of EBK quantization provides a direct connection between these classical position probability densities and the fully quantum mechanical solution with a minimum of mathematical detail.

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