Supergeneralized Runge-Lenz vector in the problem of two Coulomb or Newton centers

N. Kryukov and E. Oks
Physics Department, 206 Allison Lab, Auburn University, Auburn, Alabama 36849, USA
(Received 5 April 2012; published 29 May 2012)

A so-called two centers problem (TCP) has the following two mathematically equivalent, but physically different embodiments. The first one is the motion of an electron in the field of two stationary Coulomb centers of charges Z and Z' separated by a distance R, which is one of the most fundamental problems in quantum mechanics. The second one is the motion of a planet in the gravitational field of two stationary stars of generally different masses, which is one of the most fundamental problems in celestial mechanics. At least, two groups of authors claimed that for the TCP they derived a supergeneralized Runge-Lenz vector, whose projection on the internuclear (or interstellar) axis is conserved. In the present paper, first, we show that their claims are incorrect: the projection of their supergeneralized Runge-Lenz vector is not conserved. Second, we derive a correct supergeneralized Runge-Lenz vector whose projection on the internuclear or interstellar axis does conserve. Third, since in the literature there are several expressions for the separation constant for the TCP—the expressions not having the form of a projection of any vector on the internuclear or interstellar axis—we provide relations between those expressions and our result.

DOI: 10.1103/PhysRevA.85.054503 PACS number(s): 33.15.−e, 31.15.xg, 45.50.Pk, 95.10.Eg

I. INTRODUCTION

A so-called two centers problem (TCP) has the following two mathematically equivalent, but physically different embodiments. The first one is the motion of an electron in the field of two stationary Coulomb centers of charges Z and Z' separated by a distance R, which is one of the most fundamental problems in quantum mechanics (see, e.g., Refs. [1,2]). The second one is the motion of a planet in the gravitational field of two stationary stars of generally different masses, which is one of the most fundamental problems in celestial mechanics (see, e.g., Refs. [3,4]). The geometrical symmetry of the TCP dictates the conservation of the energy and of the projection of the angular momentum on the internuclear (or interstellar) axis. It is also well known that the TCP possesses a higher than geometrical symmetry and that there should be an additional integral of the motion. The existence of the additional integral of the motion is intimately connected with the fact that the TCP allows the separation of variables in the elliptical coordinates—the fact shown as early as in 1760 by Euler [5] (see also Ref. [6,7]).

In the limit of large R, the problem of two Coulomb centers reduces to the problem of a hydrogenic ion of the nuclear charge Z in the uniform electric field $F = Z'/R^2$, which is another fundamental problem in quantum mechanics (the corresponding celestial problem reduces to the problem of the one-center Kepler system in the uniform gravitational field). This simpler quantal problem also possesses higher than geometrical symmetry (connected with the fact that this problem allows the separation of variables in the parabolic coordinates). The corresponding integral of the motion is known as a projection of a generalized Runge-Lenz vector on the internuclear axis. The generalized Runge-Lenz vector **A** for this simpler problem, introduced by Redmond in 1964 [8], and its projection A_z on the axis $0z \| \mathbf{F}$ can be represented in the forms, respectively,

$$\mathbf{A} = \mathbf{A}_0 + (\mathbf{r} \times \mathbf{F}) \times \mathbf{r}/2, \quad A_z = A_{0z} - (x^2 + y^2)F/2 \qquad (1)$$

(atomic units are used throughout the paper). Here $\mathbf{A}_0$ is the well-known Runge-Lenz vector for one isolated Coulomb center: [1]

$$\mathbf{A}_0 = \mathbf{p} \times \mathbf{L} - Z\mathbf{r}/r. \qquad (2)$$

We note that the corresponding expressions in Redmond's paper [8] differed from Eqs. (1) and (2) by factor $1/Z$.

After Redmond introduced the generalized Runge-Lenz vector for the asymptotic case of the TCP, the challenge was to find out whether a supergeneralization of the Runge-Lenz vector is possible for the general (nonasymptotic) TCP. At least two groups of authors claimed that they accomplished this task. Namely, Krivchenkov and Liberman in 1968 [13] and Gurarie in 1992 [14] presented expressions for a supergeneralized Runge-Lenz vector and claimed that its projection on the internuclear (or interstellar) axis is conserved.

In the present paper, first, we show that their claims are incorrect: the projection of their supergeneralized Runge-Lenz vector is not conserved (despite the fact that in the limit of large R, their expressions reduce to Redmond's result). Second, we derive a correct supergeneralized Runge-Lenz vector whose projection on the internuclear or interstellar axis does conserve. Third, since in the literature there are several expressions for the separation constant for the TCP—the expressions not having the form of a projection of any vector on the internuclear or interstellar axis—we provide relations between those expressions and our result.

[1]Vector $\mathbf{A}_0$ is also called the Laplace-Runge-Lenz vector. It is interesting to note that none of these three scientists were the first to introduce this vector. Historically, it was introduced as early as in 1710 by Hermann [9,10] and Bernoulli [11] and therefore is also called the Hermann-Bernoulli vector or the Ermanno-Bernoulli vector (different just by the spelling of the first author's name, who is the same person in both cases)—more details on this history can be found in Ref. [12].

II. SUPERGENERALIZED RUNGE-LENZ VECTOR

Krivchenkov and Liberman [13] considered the TCP described by the Hamiltonian (or the Hamilton function)

$$H = p^2/2 - Z_1/r_1 - Z_2/r_2 + Z_2/R. \tag{3}$$

The charge Z_1 was placed at the origin and Z_2 at $z = R$. They presented the following expression for a supergeneralized Runge-Lenz vector:

$$\mathbf{A}^{(\mathrm{KL})} = \mathbf{p}\times\mathbf{L} - Z_1\mathbf{r}_1/r_1 + Z_2\mathbf{r}_2/r_2 + Z_2\mathbf{e_z}, \tag{4}$$

where $\mathbf{e_z}$ is the unit vector in the direction from charge Z_1 to charge Z_2. In the limit of large R, it reduces to Redmond's result from Eq. (1).

We calculated the Poisson bracket $[A^{(\mathrm{KL})},H]$ of the projection of this vector on the internuclear axis with the Hamiltonian from [13]. Surprisingly, the result was not zero:

$$[A^{(\mathrm{KL})},H] = -\left(2Z_1/r_1^3\right)\mathbf{r}\times\mathbf{L}\cdot\mathbf{e_z} - \left(2Z_2/r_2^3\right)R(xp_x + yp_y). \tag{5}$$

Thus, the projection of Krivchenkov-Liberman's vector on the internuclear axis does not conserve.

Gurarie [14] considered the TCP described by the Hamilton function

$$H = p^2/2 - Z_1/r_1 - Z_2/r_2, \tag{6}$$

where Z_1 and Z_2 are placed into $z = a$ and $z = -a$, respectively (atomic units are also used here). He presented the following expression for a supergeneralized Runge-Lenz vector:

$$\mathbf{A}^{(\mathrm{G})} = \mathbf{p}\times\mathbf{L} - Z_1(\mathbf{r} - a\mathbf{e_z})/|\mathbf{r} - a\mathbf{e_z}| - Z_2(\mathbf{r} + a\mathbf{e_z})/|\mathbf{r} + a\mathbf{e_z}|. \tag{7}$$

In the limit of large R, it reduces to Redmond's result from Eq. (1).

We calculated the Poisson bracket $[A^{(\mathrm{G})},H]$ of the projection of this vector on the interstellar axis with the Hamiltonian from [14]. Surprisingly, again the result was not zero:

$$[A^{(\mathrm{G})},H] = -2a(xp_x + yp_y)(Z_1/|\mathbf{r} - a\mathbf{e_z}|^3 - Z_2/|\mathbf{r} + a\mathbf{e_z}|^3). \tag{8}$$

Thus, the projection of Gurarie's vector on the interstellar axis does not conserve.

To derive a correct expression for the supergeneralized Runge-Lenz vector, we started from the Hamiltonian (or Hamilton function) given by Eq. (3) and followed the first few steps from Krivchenkov-Liberman's paper [13], arriving at the same expression in the elliptical coordinates as they did, for the additional conserved quantity:

$$\begin{aligned} A = {} & 1/R1/(w^2 - v^2)\left\{(w^2 - 1)(1 - v^2)\left(p_{\mathrm{w}}^2 - p_{\mathrm{v}}^2\right) \right.\\ & \left. - [(w^2 - 1)/(1 - v^2) - (1 - v^2)/(w^2 - 1)]p_\varphi^2\right\} \\ & - Z(1 + wv)/(w + v) + Z'(1 + v)(w - 1)/(w - v). \end{aligned} \tag{9}$$

Then, using the relation between the elliptical coordinates and the Cartesian coordinates,

$$\begin{aligned} & x = (R/2)[(w^2 - 1)(1 - v^2)]^{1/2}\cos\varphi, \\ & y = (R/2)[(w^2 - 1)(1 - v^2)]^{1/2}\sin\varphi, \quad z = (R/2)wv, \end{aligned} \tag{10}$$

we obtained from Eq. (9) the following: the supergeneralized Runge-Lenz vector, whose projection on the internuclear axis is really conserved, has the form

$$\begin{aligned} & \mathbf{A} = \mathbf{p}\times\mathbf{L} - L^2/R\mathbf{e_z} - Z\mathbf{r}/r - Z'(\mathbf{R} - \mathbf{r})/|\mathbf{R} - \mathbf{r}| + Z'\mathbf{e_z}, \\ & \mathbf{e_z} = \mathbf{R}/R. \end{aligned} \tag{11}$$

The Poisson bracket of the projection of the vector from Eq. (11) on the internuclear axis

$$A_z = \mathbf{p}\times\mathbf{L}\cdot\mathbf{e_z} - L^2/R - Zz/r - Z'(R - z)/|\mathbf{R} - \mathbf{r}| + Z', \tag{12}$$

with the Hamilton function from Eq. (3), vanishes indeed.

In the limit of large R, the expression from Eq. (12) reduces to the following asymptotic form:

$$(A_z)_{\mathrm{as}} = \mathbf{p}\times\mathbf{L}\cdot\mathbf{e_z} - L^2/R - Zz/r + (1/2)(x^2 + y^2)Z'/R^2. \tag{13}$$

Here the direction of the z axis is chosen from the charge Z to the charge Z'. Compared to Redmond's result from Eq. (1), there is an extra term in Eq. (13): $-L^2/R$. At first glance, this might seem puzzling. However, the Poisson bracket of $-L^2/R$ with the Hamilton function from Eq. (3) yields a term of the order of $1/R^3$. Thus, the Poisson bracket of A_{as} from Eq. (13) with the Hamilton function from Eq. (3), being calculated up to (including) terms of the order of $1/R^2$, vanishes. This resolves what might have seemed as the puzzle.

In the literature there are several expressions for the separation constant for the TCP—the expressions not having the form of a projection of any vector on the internuclear or interstellar axis. Below we provide relations between those expressions and our result.

In 1949, Erikson and Hill [15] presented the following expression for the separation constant:

$$\Omega = \mathbf{L}'\cdot\mathbf{L}'' + 2a(Z_1\cos\theta_1 - Z_2\cos\theta_2), \tag{14}$$

where $\mathbf{L}'$ and $\mathbf{L}''$ are the angular momenta of the electron with respect to Z_1 and Z_2, θ_1 and θ_2 are the angles between the radii vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ (directed from the nuclei to the electron) and the positive direction of the z axis (from Z_1 to Z_2), and $2a$ is the internuclear distance.

We found that it is related to our result from Eq. (12) as follows:

$$\Omega = R(Z' - A_z). \tag{15}$$

In Landau-Lifshitz's book of 1960 [7], there is the following expression for the separation constant:

$$\beta = \sigma^2\left(p_\rho^2 + p_\varphi^2/\rho^2\right) - M^2 + 2m\sigma(\alpha_1\cos\theta_1 + \alpha_2\cos\theta_2), \tag{16}$$

where α_1 and α_2 are the nuclear charges with the sign opposite to ours, ρ and φ are the cylindrical coordinates where the z axis is the internuclear axis, p_ρ and p_φ are the canonical momenta corresponding to these coordinates, m is the mass of the particle (in our units $m = 1$), $\mathbf{M}$ is the angular momentum of the electron with respect to the origin (which is at half the internuclear distance), 2σ is the internuclear distance, and θ_1 and θ_2 are the angles between the radii vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ and the internuclear axis measured inside the triangle made by r_1, r_2, and 2σ.

We found that it is related to our result from Eq. (12) as follows:

$$\beta = R(A_z - Z'). \tag{17}$$

In 1967, Coulson and Joseph [16] presented the following expression for the separation constant:

$$B = L^2 + a^2 p_z^2 + 2aq_1 z/r_1 - 2aq_2 z/r_2, \tag{18}$$

where q_1 and q_2 are the nuclear charges with the sign opposite to ours, **L** is the angular momentum of the particle with respect to the origin (which is at half the internuclear distance), $2a$ is the internuclear distance, r_1 and r_2 are the distances from the particle to the nuclei, z is the coordinate along the internuclear axis, and p_z is its corresponding canonical momentum.

We found that it is related to our result from Eq. (12) as follows:

$$B = R(Z' - A_z) + R^2 H/2, \tag{19}$$

where H is the Hamiltonian.

In the book by Komarov, Ponomarev, and Slavyanov published in 1976 [2], the following expression for the separation constant was presented:

$$\Lambda = L^2 + R^2 p_z^2/4 + RZ_1 z/r_1 - RZ_2 z/r_2 - R^2 H/2. \tag{20}$$

We found that it is related to our result from Eq. (12) as follows:

$$\Lambda = R(Z' - A_z). \tag{21}$$

III. CONCLUSIONS

We showed that the expressions for a supergeneralized Runge-Lenz vector presented for the TCP by Krivchenkov and Liberman [13] and by Gurarie [14] are incorrect. Its projection on the internuclear (or interstellar) axis is not conserved.

We derived a correct supergeneralized Runge-Lenz vector, whose projection on the internuclear or interstellar axis does conserve. We also analyzed the asymptotic form of the projection in the limit of large R.

Finally, since in the literature there are several expressions for the separation constant for the TCP—the expressions not having the form of a projection of any vector on the internuclear or interstellar axis—we provided relations between those expressions and our result.

The correct supergeneralized Runge-Lenz vector for the TCP that we derived should be of a general theoretical interest since the TCP is one of the most fundamental problems in physics. It can also have practical applications: for example, it can be used as a necessary tool while applying to the TCP the robust perturbation theory for degenerate states (based on the integrals of the motion) developed by Oks and Uzer [17].

ACKNOWLEDGMENTS

We would like to thank F. Robicheaux for stimulating discussions.

[1] J. D. Power, Philos. Trans. R. Soc. London, Ser. A **274**, 663 (1973).
[2] I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, *Spheroidal and Coulomb Spheroidal Functions* (Nauka, Moscow, 1976) (in Russian).
[3] C. L. Charlier, *Die Mechanik des Himmels (Celestial Mechanics)* (W. de Gruyter, Berlin, 1927).
[4] L. A. Pars, *A Treatise on Analytical Dynamics* (Heinemann, London, 1965).
[5] L. Euler, *Mem. De Berlin,* (1760), p. 228.
[6] M. Born, *Vorlesungen über Atommechanik (The Mechanics of the Atom)* (Springer, Berlin, 1925).
[7] L. D. Landau and E. M. Lifshitz, *Mechanics* (Pergamon, Oxford, 1960).
[8] P. J. Redmond, Phys. Rev. **133**, B1352 (1964).
[9] J. Hermann, Giornale de Letterati D'Italia **2**, 447 (1710).
[10] J. Hermann, *Histoires de L'Academie Royale des Sciences avec le Memoires de Mathematique et Physique* [Paris (1710), 1712], pp. 102, 519.
[11] J. I. Bernoulli, *Histoires de L'Academie Royale des Sciences avec le Memoires de Mathematique et Physique* [Paris (1710), 1712], pp. 523, 685.
[12] H. Goldstein, Am. J. Phys. **44**, 1123 (1976).
[13] V. D. Krivchenkov and M. A. Liberman, Russ. Phys. J., **11**, 14 (1968).
[14] D. Gurarie, in *Symmetries and Laplacians: Introduction to Harmonic Analysis, Group Representations and Applications,* North Holland Mathematics Studies Vol. 174 (North Holland, Amsterdam, 1992), p. 390.
[15] H. A. Erikson and E. L. Hill, Phys. Rev. **75**, 29 (1949).
[16] C. A. Coulson and A. Joseph, Int. J. Quantum Chem. **1**, 337 (1967).
[17] E. Oks and T. Uzer, Europhys. Lett. **49**, 554 (2000).