Semiclassical wave functions and semiclassical dynamics for the Kepler/Coulomb problem

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Abstract

We investigate the semiclassical Kepler/Coulomb problem using the classical constants of the motion in the framework of Nelson's stochastic mechanics. This is done by considering the eigenvalue relations for a family of coherent states (known as the atomic elliptic states) whose wave functions are concentrated on the elliptical orbit corresponding to the associated classical problem. We show that these eigenvalue relations lead to identities for the semiclassical energy, angular momentum and Hamilton-Lenz-Runge vectors in the elliptical case. These identities are then extended to include the cases of circular, parabolic and hyperbolic motions. We show that in all cases the semiclassical wave function is determined by our identities and so our identities can be seen as defining a semiclassical Kepler/Coulomb problem. The results are interpreted in terms of two dynamical systems: one a complex valued solution to the classical mechanics for a Coulomb potential and the other the drift field for a semiclassical Nelson diffusion.

1 Introduction

Consider the Hamiltonian for a classical particle of unit mass driven by a Coulomb potential,

$$H = \frac{1}{2}|\boldsymbol{p}|^2 - \frac{\mu}{|\boldsymbol{x}|},$$

where $\mu > 0$ and $\boldsymbol{x} = (x_1, x_2, x_3)$, $\boldsymbol{p} = (p_1, p_2, p_3)$ denote respectively the position and momentum in Cartesian coordinates. The classical motion of such a system is characterised by seven constants: the energy E, angular momentum $\boldsymbol{l}'$ and Hamilton-Lenz-Runge vector $\boldsymbol{a}'$ given by,

$$E = \frac{|\boldsymbol{p}|^2}{2} - \frac{\mu}{|\boldsymbol{x}|}, \qquad \boldsymbol{l}' = \boldsymbol{x} \wedge \boldsymbol{p}, \qquad \boldsymbol{a}' = \boldsymbol{p} \wedge \boldsymbol{l}' - \frac{\mu \boldsymbol{x}}{|\boldsymbol{x}|}, \tag{1}$$

subject to the constraint $\boldsymbol{l}' \cdot \boldsymbol{a}' = 0$. (Note that we use the prime to denote that these are the classical quantities and reserve $\boldsymbol{l}$ and $\boldsymbol{a}$ for their semiclassical versions which will be discussed later.) The orbits for such a system are conic sections with eccentricity e and semilatus rectum Λ determined by Newton's famous formulae,

$$e = \sqrt{1 + \frac{2\Lambda E}{\mu}}, \qquad \Lambda = \frac{|\boldsymbol{l}'|^2}{\mu}. \tag{2}$$

Indeed it follows in the bound case ($E < 0$) that if the axes are aligned so that the motion takes place in the plane $x_3 = 0$ with the semi-major axis of the ellipse aligned with the x_1 axis then,

$$a'_1 = \mu e, \qquad a'_2 = a'_3 = 0, \qquad l'_1 = l'_2 = 0, \qquad l'_3 = \mu\sqrt{\frac{1-e^2}{-2E}}, \tag{3}$$

where $\boldsymbol{a}' = (a'_1, a'_2, a'_3)$ and $\boldsymbol{l}' = (l'_1, l'_2, l'_3)$.

In this paper we will investigate a semiclassical version of this system which will in particular lead to a natural complex extension of the equations (3).

Consider the quantum mechanics for a particle of unit mass with the corresponding Hamiltonian,

$$H = \frac{1}{2}|\boldsymbol{P}|^2 - \frac{\mu}{|\boldsymbol{Q}|},$$

where $\boldsymbol{Q} = (Q_1, Q_2, Q_3)$ and $\boldsymbol{P} = (P_1, P_2, P_3)$ denote the quantum position and momentum operators respectively. We will investigate the semiclassical mechanics which can be derived from a family of coherent states for this Hamiltonian. The states in question are the *atomic elliptic states* [1] with eccentricity $e = \sin\theta \in (0,1)$ whose wave functions have the Cartesian representation [2],

$$\psi_{n,\theta}(\boldsymbol{x}) := C \exp\left(-\frac{n\mu}{\lambda^2}|\boldsymbol{x}|\right) L_{n-1}(n\nu(\boldsymbol{x})), \tag{4}$$

for some suitable normalisation constant $C > 0$, where L_n is a Laguerre polynomial and

$$\nu(\boldsymbol{x}) = \frac{\mu}{\lambda^2}\left(|\boldsymbol{x}| - \frac{x_1}{e} - i\frac{x_2}{e}\sqrt{1-e^2}\right), \qquad \boldsymbol{x} = (x_1, x_2, x_3). \tag{5}$$

For each fixed value of $e = \sin\theta$, the wave function $\psi_{n,\theta}$ defines a stationary state for H which satisfies,

$$H\psi_{n,\theta} = E_n\psi_{n,\theta}, \qquad E_n = -\frac{\mu^2}{2\lambda^2}, \qquad \lambda = n\hbar,$$

and also has the best possible localisation on the elliptical orbit from the corresponding classical problem with energy E_n and prescribed eccentricity $e = \sin\theta$. That is, the wave function $\psi_{n,\theta}$ is concentrated on an ellipse (the *Kepler ellipse*) with eccentricity $e = \sin\theta$, semilatus rectum $\Lambda = \lambda^2(1-e^2)/\mu$ and semimajor axis λ^2/μ parallel to the x_1 axis in the plane $x_3 = 0$ with one focus at the origin. The semiclassical behaviour of this state has previously been analysed [3, 4, 5] in the framework of Nelson's stochastic mechanics [6].

In Nelson's theory the state $\psi_{n,\theta}$ is associated to a diffusion process,

$$\mathrm{d}\boldsymbol{X}_t = \boldsymbol{b}^{n,\theta}(\boldsymbol{X}_t, t)\,\mathrm{d}t + \sqrt{\hbar}\,\mathrm{d}\boldsymbol{B}_t, \tag{6}$$

where $\boldsymbol{B}_t$ is a three dimensional Brownian motion process and the drift is given by $\boldsymbol{b}^{n,\theta} = \operatorname{Re}\boldsymbol{Z}^{n,\theta} - \operatorname{Im}\boldsymbol{Z}^{n,\theta}$ with $\boldsymbol{Z}^{n,\theta} = -i\hbar\nabla\ln\psi_{n,\theta}$ (there are singularities here at the nodes of $\psi_{n,\theta}$ [7]). The Nelson diffusion $\boldsymbol{X}_t$ defined by (6) can be shown to satisfy the *Nelson-Newton law*, a stochastic version of Newton's second law,

$$\frac{1}{2}(D_+D_- + D_-D_+)\boldsymbol{X}_t = -\frac{\mu\boldsymbol{X}_t}{|\boldsymbol{X}_t|^3}, \tag{7}$$

where the left hand side of (7) is thought of as the *stochastic acceleration* defined in terms of mean conditioned derivatives,

$$D_\pm f(\boldsymbol{X}_t) = \lim_{h\to 0}\mathbb{E}\left(\left.\frac{f(\boldsymbol{X}_{t\pm h}) - f(\boldsymbol{X}_t)}{\pm h}\right|\boldsymbol{X}_t\right).$$

This gives a theory which is mathematically equivalent to the Schrödinger equation (the diffusion $\boldsymbol{X}_t$ is uniquely determined by the wave function) but the physical significance of the diffusion process is controversial [8, 9].

By considering the correspondence limit of the complex vector $\boldsymbol{Z}^{n,\theta}$ ($n \to \infty$ and $\hbar \to 0$ with $\lambda = n\hbar$ fixed) we can define [3],

$$\boldsymbol{Z}(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\,\hbar\to 0\\ n\hbar=\lambda}} \boldsymbol{Z}^{n,\theta}(\boldsymbol{x}) = \frac{i\mu}{2\lambda}\,(1+\gamma)\,\frac{\boldsymbol{x}}{|\boldsymbol{x}|} + \frac{\mu}{2\lambda e}\,(1-\gamma)\,(i, -\sqrt{1-e^2}, 0), \tag{8}$$

where

$$\gamma(\boldsymbol{x}) = 1 - 2 \lim_{\substack{n\to\infty,\,\hbar\to 0\\ n\hbar=\lambda}} \frac{L'_{n-1}(n\nu(\boldsymbol{x}))}{L_{n-1}(n\nu(\boldsymbol{x}))} = \sqrt{1-\frac{4}{\nu(\boldsymbol{x})}}. \tag{9}$$

Moreover we can then define a semiclassical elliptic wave function given by (up to some normalising constant),

$$\psi_{\text{s.c.}}(\boldsymbol{x}) \quad = \nu(\boldsymbol{x})^{\lambda/\hbar}(1+\gamma(\boldsymbol{x}))^{2\lambda/\hbar} \exp\left(-\tfrac{\mu}{\lambda\hbar}|\boldsymbol{x}| + \tfrac{\lambda}{2\hbar}(1-\gamma(\boldsymbol{x}))\nu(\boldsymbol{x})\right),$$

which satisfies $\boldsymbol{Z} = -i\hbar\nabla \ln \psi_{\text{s.c.}}$. We can then write,

$$\psi_{\text{s.c.}} = \exp\left(\hbar^{-1}(R+iS)\right)$$

for real valued functions $R, S : \mathbb{R}^3 \to \mathbb{R}$ giving $\boldsymbol{Z} = \nabla S - i\nabla R$. In turn, following Nelson, we can define the *Keplerian diffusion* $\boldsymbol{X}_t^\epsilon$ by,

$$\mathrm{d}\boldsymbol{X}_t^\epsilon = \boldsymbol{b}(\boldsymbol{X}_t^\epsilon)\,\mathrm{d}t + \epsilon\,\mathrm{d}\boldsymbol{B}_t, \quad \boldsymbol{b} = \operatorname{Re}\boldsymbol{Z} - \operatorname{Im}\boldsymbol{Z} = \nabla R + \nabla S, \tag{10}$$

where $\epsilon = \sqrt{\hbar}$. Again there are difficulties associated with the nodal set of $\psi_{n,\theta}$ [3, 4]. Nevertheless, this Keplerian diffusion can be viewed as a semiclassical description of the position of the electron in a hydrogen atom in the atomic elliptic state.

In this paper we investigate the relation between the semiclassical vector field $\boldsymbol{Z}$ (which determines both the drift field $\boldsymbol{b}$ and the wave function $\psi_{\text{s.c.}}$) and the constants of the classical motion (1). If we define the corresponding quantum mechanical angular momentum and Hamilton-Lenz-Runge operators by,

$$\boldsymbol{L} = \boldsymbol{Q} \wedge \boldsymbol{P}, \qquad \boldsymbol{A} = \frac{1}{2}\,(\boldsymbol{P}\wedge\boldsymbol{L} - \boldsymbol{L}\wedge\boldsymbol{P}) - \frac{\mu\boldsymbol{Q}}{|\boldsymbol{Q}|},$$

then we can define (avoiding the nodes of $\psi_{n,\theta}$) the corresponding semiclassical quantities as functions $\boldsymbol{a}, \boldsymbol{l} : \mathbb{R}^3 \to \mathbb{C}^3$ given by the pointwise limits,

$$\boldsymbol{l}(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\, \hbar\to 0\\ n\hbar=\lambda}} \frac{\boldsymbol{L}\psi_{n,\theta}(\boldsymbol{x})}{\psi_{n,\theta}(\boldsymbol{x})}, \qquad \boldsymbol{a}(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\, \hbar\to 0\\ n\hbar=\lambda}} \frac{\boldsymbol{A}\psi_{n,\theta}(\boldsymbol{x})}{\psi_{n,\theta}(\boldsymbol{x})}.$$

It follows that,

$$\boldsymbol{l} = \boldsymbol{x} \wedge \boldsymbol{Z}, \qquad \boldsymbol{a} = \boldsymbol{Z} \wedge (\boldsymbol{x} \wedge \boldsymbol{Z}) - \frac{\mu \boldsymbol{x}}{|\boldsymbol{x}|}.$$

The operators $\boldsymbol{L}$ and $\boldsymbol{A}$ are generators of $SO(4)$, and using the $SO(4)$ symmetry of H to establish the eigenvalue relations of the atomic elliptic state we show that the semiclassical versions of the identities (3) for an ellipse of eccentricity $e = \sin\theta$ are given by the complex equations,

$$a_1 + i a_2\sqrt{1-e^2} = \mu e, \quad l_1 + i l_2\sqrt{1-e^2} = 0, \tag{11}$$

$$\frac{\mu}{\lambda} l_3 - i a_2 e = \mu\sqrt{1-e^2}, \qquad a_3 - i\tfrac{\mu}{\lambda} l_2 e = 0, \tag{12}$$

where $\boldsymbol{a} = (a_1, a_2, a_3)$ and $\boldsymbol{l} = (l_1, l_2, l_3)$. Equations (11) and (12) are thus identities for $\boldsymbol{a}$ and $\boldsymbol{l}$ in the semiclassical dynamics.

In the case that there exists a region $D \subset \mathbb{R}^3$ such that $a_i(\boldsymbol{x}), l_i(\boldsymbol{x}) \in \mathbb{R}$ for $i = 1, 2, 3$ for all $\boldsymbol{x} \in D$, then these reduce to the classical identities,

$$l_1(\boldsymbol{x}) = l_2(\boldsymbol{x}) = 0, \quad l_3(\boldsymbol{x}) = \lambda\sqrt{1-e^2}, \quad a_1(\boldsymbol{x}) = \mu e, \quad a_2(\boldsymbol{x}) = a_3(\boldsymbol{x}) = 0,$$

which are consistent with (3) so that in this case $\boldsymbol{a}(\boldsymbol{x})$ and $\boldsymbol{l}(\boldsymbol{x})$ are the classical constants describing the elliptical orbit of eccentricity e on the domain D. That is,

$$\boldsymbol{a}(\boldsymbol{x}) = \boldsymbol{a}', \qquad \boldsymbol{l}(\boldsymbol{x}) = \boldsymbol{l}',$$

for all $\boldsymbol{x} \in D$. This is indeed the case on the Kepler ellipse where $|\mathrm{Im}\, \boldsymbol{Z}| = |\nabla R| = 0$.

Having established equations (11), (12) together with a semiclassical version of the energy equation,

$$\frac{1}{2}|\boldsymbol{Z}|^2 - \frac{\mu}{|\boldsymbol{x}|} = -\frac{\mu^2}{2\lambda^2}, \tag{13}$$

we will consider their natural extension to the circular, parabolic and hyperbolic situations and we show that the semiclassical vector $\boldsymbol{Z}$ and hence the semiclassical wave functions $\psi_{\text{s.c.}}$ can be determined solely from these identities. Thus the equations (11), (12) and (13) and their generalisations can be viewed as defining a semiclassical version of Keplerian motion. In the circular case the vector $\boldsymbol{Z}$ is uniquely determined by these equations, but in all other cases there are two possible solutions. Moreover, for the circular orbit ($e = 0$) it should be noted that our identities reduce to,

$$a_1 + ia_2 = l_1 + il_2 = 0, \qquad l_3 = \lambda, \qquad a_3 = 0,$$

which recapitulate the eigenvalue and ladder identities for the circular wave function $\psi_{n,n-1,n-1}$ where ψ_{nlm} denotes the standard nodal wave function for the hydrogen atom which satisfies the relations,

$$L_3\psi_{nlm} = m\hbar\psi_{nlm}, \qquad |\boldsymbol{L}|^2\psi_{nlm} = l(l+1)\hbar^2\psi_{nlm}, \qquad H\psi_{nlm} = E_n\psi_{nlm},$$

where $n, l, m \in \mathbb{Z}$ with $-l \leq m \leq l$ and $0 \leq l \leq n-1$.

We interpret our results in terms of two classical mechanical systems. First we consider the deterministic limit of the semiclassical Nelson diffusion (10),

$$\dot{\boldsymbol{X}}^0(t) = \boldsymbol{b}(\boldsymbol{X}^0(t)), \qquad \dot{\boldsymbol{X}}^0(0) = \boldsymbol{b}(\boldsymbol{x}_0), \qquad \boldsymbol{X}^0(0) = \boldsymbol{x}_0,$$

which acts as an underlying classical system for the Hamiltonian,

$$H(\boldsymbol{x}, \boldsymbol{p}) = \frac{|\boldsymbol{p}|^2}{2} - \frac{\mu}{|\boldsymbol{x}|} - |\mathrm{Im}\,\boldsymbol{Z}(\boldsymbol{x})|^2.$$

In this system for the bound energy case (elliptic and circular) it has previously been shown [4] that under natural assumptions on the density the motion converges towards Keplerian motion on the Kepler ellipse/circle. For the scattering cases all trajectories are Keplerian parabolas/hyperbolas. Interestingly here whilst the two different solutions for $\boldsymbol{Z}$ are physically significant in the parabolic and hyperbolic case, only one appears physically relevant in the elliptic case (see Figure 2). We also consider the classical mechanics for the Coulomb potential in the complex phase space $\mathbb{C}^6$ and show that the vector $\boldsymbol{Z}$ determines the momentum field for the system governed by the Hamiltonian,

$$H(\boldsymbol{x}, \boldsymbol{Z}) = \frac{|\boldsymbol{Z}|^2}{2} - \frac{\mu}{|\boldsymbol{x}|},$$

under the constraint that the energy of the system is real. Such complex classical mechanical systems have generated much interest recently through their relation to $\mathcal{PT}$ symmetric quantum mechanics [10, 11, 12].

Moreover there is a natural relation between these classical mechanical systems and the Hamilton-Jacobi equations used in Maslov's approach to the semiclassical limit of the Schrödinger equation [13, 14].

The paper is structured as follows:-

In Section 2 we discuss relevant properties of $SO(4)$ and the quantum Kepler/Coulomb problem. In Section 3 we introduce the atomic elliptic state and derive the key eigenvalue relations (Theorem 3) and derive their semiclassical versions (Theorem 4). In Section 4 we take the semi-classical equations (Table 1) as fundamental and show that they determine the semi-classical wave functions and Nelson diffusions (Theorem 7). We conclude with a discussion of the dynamics and Hamilton-Jacobi equations associated with $\boldsymbol{b}$ and $\boldsymbol{Z}$.

2 The quantum Kepler/Coulomb problem

Recall that H denotes the Hamiltonian for the quantum Kepler/Coulomb problem. We define the quantum angular momentum $\boldsymbol{L} = (L_1, L_2, L_3) = \boldsymbol{Q} \wedge \boldsymbol{P}$ with $|\boldsymbol{L}|^2 = L_1^2 + L_2^2 + L_3^2$ and the quantum Hamilton-Lenz-Runge vector $\boldsymbol{A} = (A_1, A_2, A_3) = \frac{1}{2}(\boldsymbol{P} \wedge \boldsymbol{L} - \boldsymbol{L} \wedge \boldsymbol{P}) - \frac{\mu \boldsymbol{Q}}{|\boldsymbol{Q}|}$. As is well known, the following holds:

Theorem 1. *The operators $\boldsymbol{L}$, $\boldsymbol{A}$ and H satisfy,*

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \quad [L_i, A_j] = i\hbar\epsilon_{ijk}A_k, \quad [A_i, A_j] = -2i\hbar\epsilon_{ijk}HL_k, \tag{14}$$

and,

$$[H, L_j] = [H, A_j] = 0, \quad |\boldsymbol{A}|^2 = 2H(|\boldsymbol{L}|^2 + \hbar^2) + \mu^2, \quad \boldsymbol{L} \cdot \boldsymbol{A} = \boldsymbol{A} \cdot \boldsymbol{L} = 0.$$

If we define,

$$\boldsymbol{J}^{\pm} = \frac{1}{2}\left(\boldsymbol{L} \pm \frac{\boldsymbol{A}}{\sqrt{-2H}}\right) P_H,$$

where P_H denotes the projection onto the eigenfunctions of the negative spectrum of the Hamiltonian H, then,

$$[J_i^{\pm}, J_j^{\pm}] = i\hbar\epsilon_{ijk}J_k^{\pm}, \quad [J_i^{\pm}, J_j^{\mp}] = 0, \quad |\boldsymbol{J}^{\pm}|^2 = -\frac{1}{4}\left(\hbar^2 + \frac{\mu^2}{2H}\right) P_H. \tag{15}$$

Proof. See Thirring [15]. □

If we define a new observable $\tilde{\boldsymbol{A}} = (-2H)^{-1/2}\boldsymbol{A}P_H$, then (14) yields,

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \quad [L_i, \tilde{A}_j] = i\hbar\epsilon_{ijk}\tilde{A}_k, \quad [\tilde{A}_i, \tilde{A}_j] = i\hbar\epsilon_{ijk}L_k, \tag{16}$$

which are the generators of $SO(4)$. Indeed, borrowing notation from [1], we can construct a four dimensional angular momentum operator,

$$\mathcal{L}_{ij} = \epsilon_{ijk}L_k, \quad \mathcal{L}_{i4} = -\mathcal{L}_{4i} = \tilde{A}_i, \quad \mathcal{L}_{44} = 0, \quad i, j, k \in \{1, 2, 3\},$$

which satisfies the commutation relations,

$$[\mathcal{L}_{ij}, \mathcal{L}_{ik}] = i\hbar\mathcal{L}_{jk}, \quad i, j, k \in \{1, 2, 3, 4\}, \tag{17}$$

where $[\mathcal{L}_{ij}, \mathcal{L}_{kl}] = 0$ if i, j, k, l are all distinct. Considering the rotations generated by these operators gives the following result:

Lemma 1. *Define,*

$$\mathcal{L}_{ijk}(\theta) = \exp\left(-\frac{i\theta}{\hbar}\mathcal{L}_{ik}\right)\mathcal{L}_{ij}\exp\left(\frac{i\theta}{\hbar}\mathcal{L}_{ik}\right),$$

where $i, j, k \in \{1, 2, 3, 4\}$ all distinct. Then,

$$\mathcal{L}_{ijk}(\theta) = \mathcal{L}_{ij}\cos\theta - \mathcal{L}_{jk}\sin\theta.$$

Proof. It follows from Stone's Theorem and equation (17) that for suitable ψ,

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\mathcal{L}_{ijk}(\theta)\psi \quad = \tfrac{i}{\hbar}\exp\left(-\tfrac{i\theta}{\hbar}\mathcal{L}_{ik}\right)[\mathcal{L}_{ij}, \mathcal{L}_{ik}]\exp\left(\tfrac{i\theta}{\hbar}\mathcal{L}_{ik}\right)\psi = \mathcal{L}_{kji}(-\theta)\psi.$$

Thus,

$$\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}\mathcal{L}_{ijk}(\theta)\psi = -\mathcal{L}_{ijk}(\theta)\psi,$$

giving the result. □

More explicitly:-

Corollary 1. *For $j, k \in \{1, 2, 3\}$ with $j \neq k$,*

$$\begin{aligned}
\exp\left(-\frac{i\theta}{\hbar}\tilde{A}_k\right)\tilde{A}_j\exp\left(\frac{i\theta}{\hbar}\tilde{A}_k\right) &= \tilde{A}_j\cos\theta - \epsilon_{jkl}L_l\sin\theta, \\
\exp\left(-\frac{i\theta}{\hbar}\tilde{A}_k\right)L_j\exp\left(\frac{i\theta}{\hbar}\tilde{A}_k\right) &= L_j\cos\theta - \epsilon_{jkl}\tilde{A}_l\sin\theta.
\end{aligned}$$

We now define for each $\theta \in [0, \pi/2]$ and $j = 1, 2, 3$,

$$\tilde{A}_j(\theta) := \exp\left(-\frac{i\theta}{\hbar}\tilde{A}_2\right)\tilde{A}_j \exp\left(\frac{i\theta}{\hbar}\tilde{A}_2\right)$$
$$\tilde{L}_j(\theta) := \exp\left(-\frac{i\theta}{\hbar}\tilde{A}_2\right)L_j \exp\left(\frac{i\theta}{\hbar}\tilde{A}_2\right).$$

Corollary 2. *For each fixed $\theta \in [0, \pi/2]$,*

$$[\tilde{L}_i(\theta), \tilde{L}_j(\theta)] = i\hbar\epsilon_{ijk}\tilde{L}_k(\theta),$$

$$[\tilde{L}_i(\theta), \tilde{A}_j(\theta)] = i\hbar\epsilon_{ijk}\tilde{A}_k(\theta),$$

$$[\tilde{A}_i(\theta), \tilde{A}_j(\theta)] = i\hbar\epsilon_{ijk}\tilde{L}_k(\theta).$$

That is for each fixed $\theta \in [0, \pi/2]$ the operators $\tilde{L}_j(\theta), \tilde{A}_j(\theta)$ with $j = 1, 2, 3$ are generators for $SO(4)$. These operators are key to the construction of the atomic elliptic state which we now discuss.

3 The atomic elliptic state

We define $|nlm\rangle$ such that,

$$L_3|nlm\rangle = m\hbar|nlm\rangle, \tag{18}$$
$$|\boldsymbol{L}|^2|nlm\rangle = l(l+1)\hbar^2|nlm\rangle, \tag{19}$$
$$H|nlm\rangle = E_n|nlm\rangle, \tag{20}$$
$$|\boldsymbol{J}^{\pm}|^2|nlm\rangle = (n^2-1)\hbar^2|nlm\rangle, \tag{21}$$

where $n, l, m \in \mathbb{Z}$ with $-l \leq m \leq l$ and $0 \leq l \leq n-1$. We also define the state $|jm^+m^-\rangle$ such that,

$$|\boldsymbol{J}^{\pm}|^2|jm^+m^-\rangle = j(j+1)\hbar^2|jm^+m^-\rangle, \tag{22}$$
$$J_3^{\pm}|jm^+m^-\rangle = m^{\pm}\hbar|jm^+m^-\rangle, \tag{23}$$
$$H|jm^+m^-\rangle = -\frac{\mu^2}{2\hbar^2(1+2j)^2}|jm^+m^-\rangle, \tag{24}$$

where $j, m^+, m^- \in \mathbb{Z}/2$ with $-j \leq m^+, m^- \leq j$. These two states are connected via the Clebsch-Gordon coefficients [16],

$$|nlm\rangle = \sum_{m^+,m^-}\langle jm^+m^-|nlm\rangle|jm^+m^-\rangle, \tag{25}$$

where $j = \frac{1}{2}(n-1)$ and $m = m^+ + m^-$.

It is well known that the state $|\mathrm{Circ}(n)\rangle := |n, l = n-1, m = n-1\rangle$ is concentrated on a circle [15] as is encapsulated in the following relations:-

Theorem 2. *The circular state satisfies the eigenvalue relations,*

$$\begin{aligned} H|\mathrm{Circ}(n)\rangle &= E_n|\mathrm{Circ}(n)\rangle, \\ L_3|\mathrm{Circ}(n)\rangle &= \hbar(n-1)|\mathrm{Circ}(n)\rangle, \\ \tilde{A}_3|\mathrm{Circ}(n)\rangle &= 0, \\ \Big(L_1 + iL_2\Big)|\mathrm{Circ}(n)\rangle &= 0, \\ \Big(\tilde{A}_1 + i\tilde{A}_2\Big)\,|\mathrm{Circ}(n)\rangle &= 0. \end{aligned}$$

Proof. These are either obvious or follow from observing that equation (25) yields,

$$|\mathrm{Circ}(n)\rangle = C|j, m^+ = j, m^- = j\rangle, \qquad j = \frac{1}{2}(n-1), \tag{26}$$

for some constant phase factor C. □

Corollary 3. *Let $\langle\cdot\rangle_n$ denote the mean in the circular state. Then,*

$$\langle L_1\rangle_n = \langle L_2\rangle_n = 0, \quad \langle L_3\rangle_n = \hbar(n-1), \quad \langle\tilde{A}_1\rangle_n = \langle\tilde{A}_2\rangle_n = \langle\tilde{A}_3\rangle_n = 0,$$

where $\langle\cdot\rangle_n$ denotes the mean value in the state $|\mathrm{Circ}(n)\rangle$.

In the correspondence limit these relations correspond to equations (3) and hence characterise circular motion on the classical orbit with eccentricity $e = 0$ and energy $-\frac{\mu^2}{2\lambda^2}$.

We now briefly explain the derivation of the atomic elliptic state by considering the coherent state representation of $SO(4) = SO(3) \otimes SO(3)$ [1]. Recall that if $T(g)$ is a unitary representation of $SO(4)$ acting on the state space of our system where $g \in SO(4)$ then a generalised coherent state representation is given by $T(g)|\psi\rangle$ for some fixed initial state $|\psi\rangle$ [17]. Consider an angular momentum operator $\boldsymbol{J}$ with corresponding eigenstate $|jm\rangle$ such that,

$$J_3|jm\rangle = \hbar m|jm\rangle, \qquad |\boldsymbol{J}|^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle,$$

where $j = 0, \frac{1}{2}, 1, \ldots$ and $m = -j, -j+1, \ldots, j$. For a fixed j the state $|jj\rangle$ has minimal uncertainty for the uncertainty principle $\Delta J_1 \Delta J_2 \geq \frac{\hbar}{2}|\langle J_3\rangle|$ and so can be used to construct a system of minimal uncertainty coherent states $|j\boldsymbol{u}\rangle$ for $SO(3)$ as,

$$|j\boldsymbol{u}\rangle := \exp\left(-\frac{i\theta}{\hbar}(\boldsymbol{u}\wedge\boldsymbol{k})\cdot\boldsymbol{J}\right)|jj\rangle,$$

where $\boldsymbol{u}$ is any unit vector, $\theta = \angle(\boldsymbol{u},\boldsymbol{k})$ and $(\boldsymbol{i},\boldsymbol{j},\boldsymbol{k})$ are the Cartesian coordinate axes. If we fix two arbitrary unit vectors $\boldsymbol{u}^{\pm}$ then we can write $\boldsymbol{u}^{\pm} = \pm\sin\theta\boldsymbol{i} + \cos\theta\boldsymbol{k}$ for some appropriate choice of axes. Considering the pair of commuting angular momenta $\boldsymbol{J}^{\pm}$, we can form a coherent state representation for $SO(4)$ as $|j^+\boldsymbol{u}^+\rangle\otimes|j^-\boldsymbol{u}^-\rangle$ where it follows from (15) that $j^{\pm} = \frac{1}{2}(n-1)$. We can then define,

$$\begin{aligned}|\mathrm{Elliptic}(n,\theta)\rangle &= |j^+\boldsymbol{u}^+\rangle\otimes|j^-\boldsymbol{u}^-\rangle\\ &= \exp\left(\tfrac{i\theta}{\hbar}(J_2^- - J_2^+)\right)|j,m^+=j,m^-=j\rangle\\ &= \exp\left(-\tfrac{i\theta}{\hbar}\tilde{A}_2\right)|j,m^+=j,m^-=j\rangle,\end{aligned}$$

where $j = \frac{1}{2}(n-1)$. It follows from (26) that up to some phase factor, we can define the atomic elliptic wave function as,

$$\begin{aligned}\psi_{n,\theta}(\boldsymbol{x}) &:= \exp\left(-\tfrac{i\theta}{\hbar}\tilde{A}_2\right)\psi_{n,n-1,n-1}(\boldsymbol{x})\\ &= C\exp\left(-\tfrac{n\mu}{\lambda^2}|\boldsymbol{x}|\right)L_{n-1}(n\nu(\boldsymbol{x})),\end{aligned}\tag{27}$$

where $\psi_{nlm}(\boldsymbol{x}) = \langle\boldsymbol{x}|nlm\rangle$. The Cartesian representation for this state was first derived in [2] using the Kustaanheimo-Stiefel transformation.

As is well known the states ψ_{nlm} form a complete orthonormal family of eigenfunctions and so any wave function of the form,

$$\exp\left(-\frac{i\theta}{\hbar}\tilde{A}_2\right)\psi_{n',l',m'}$$

for some n', l', m' is orthogonal to the atomic elliptic state $\psi_{n,\theta}$ as long as $(n', l', m') \neq (n, n-1, n-1)$. Thus the atomic elliptic states are not complete in $L^2(\mathbb{R}^3)$.

Theorem 3. *The elliptic state $\psi_{n,\theta}$ satisfies:-*

$$H\psi_{n,\theta} = E_n\psi_{n,\theta},$$

$$\begin{aligned}
\tilde{L}_3(\theta)\psi_{n,\theta} &= \left(L_3\cos\theta + \tilde{A}_1\sin\theta\right)\psi_{n,\theta} = \hbar(n-1)\psi_{n,\theta}, \\
\tilde{A}_3(\theta)\psi_{n,\theta} &= \left(\tilde{A}_3\cos\theta + L_1\sin\theta\right)\psi_{n,\theta} = 0, \\
\left(\tilde{L}_1(\theta) + i\tilde{L}_2(\theta)\right)\psi_{n,\theta} &= \left(L_1\cos\theta + iL_2 - \tilde{A}_3\sin\theta\right)\psi_{n,\theta} = 0, \\
\left(\tilde{A}_1(\theta) + i\tilde{A}_2(\theta)\right)\psi_{n,\theta} &= \left(\tilde{A}_1\cos\theta + i\tilde{A}_2 - L_3\sin\theta\right)\psi_{n,\theta} = 0.
\end{aligned}$$

Proof. Follows from Theorem 2 and Corollary 1. □

The eigenvalue relations here should be compared with those for the circular state given in Corollary 2. We note that this theorem gives the following result from [1]:-

Corollary 4. *Let $\langle\cdot\rangle_{n,\theta}$ denote the mean in the state $\psi_{n,\theta}$. Then,*

$$\begin{aligned}
\langle L_1\rangle_{n,\theta} &= \langle L_2\rangle_{n,\theta} = 0, \\
\langle L_3\rangle_{n,\theta} &= \hbar(n-1)\cos\theta, \\
\langle \tilde{A}_2\rangle_{n,\theta} &= \langle \tilde{A}_3\rangle_{n,\theta} = 0, \\
\langle \tilde{A}_1\rangle_{n,\theta} &= \hbar(n-1)\sin\theta.
\end{aligned}$$

In the correspondence limit these relations again correspond to equations (3) and hence characterise motion on the classical elliptic orbit of eccentricity e and energy $-\frac{\mu^2}{2\lambda^2}$ whose semi-major axis is aligned with the x_1 axis.

We can now determine identities to be satisfied by semiclassical versions of $\boldsymbol{L}$ and $\boldsymbol{A}$.

Lemma 2. *Let $N_{n,\theta}$ denote the nodal set of the wave function $\psi_{n,\theta}$ and define,*

$$\Sigma_\theta = \left\{\boldsymbol{x} \in \mathbb{R}^3 : \quad x_2 = 0, \quad 0 \le \frac{\mu}{\lambda^2}\left(|\boldsymbol{x}| - \frac{x_1}{\sin\theta}\right) < 4\right\}.$$

Then for a fixed θ, the set Σ_θ is the smallest connected set such that

$$N_\theta := \bigcup_{n\in\mathbb{N}} N_{n,\theta} \subset \Sigma_\theta.$$

Moreover, N_θ is dense in Σ_θ.

Proof. The Laguerre polynomial L_{n-1} has $(n-1)$ zeros which are all positive. Thus, if z_j with $j = 1, \ldots n-1$ denote the $n-1$ zeros of the Laguerre

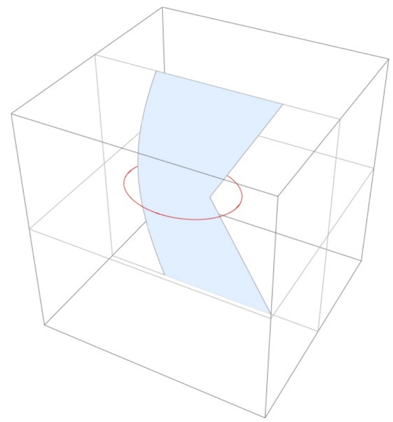


Figure 1: The surface Σ_θ for $\sin\theta = 0.5$ with $\lambda = \mu = 1$ together with the corresponding Kepler ellipse (based on Figure 5 in [3]).

polynomial L_{n-1} arranged in increasing order then the nodal set is defined by the equations,

$$z_j = \frac{n\mu}{\lambda^2}\left(|\boldsymbol{x}| - \frac{x_1}{\sin\theta}\right), \qquad x_2 = 0.$$

Moreover, [18] Theorem 6.31.2 gives,

$$0 < z_j < 2n - 1 + \left((2n-1)^2 + 1/4\right)^{1/2} < 4n,$$

and so we find that the nodal set for a fixed n is contained within the region Σ_θ. Finally [18] Theorem 6.31.3 gives the bound $z_1 \leq \frac{3}{2n-1}$ and [19] gives the bound $4n - 16\sqrt{2n} < z_{n-1}$ so that Σ_θ is the smallest connected set containing the entire nodal set for all $n \in \mathbb{Z}$. Finally in the limit $n \to \infty$ the set $\{z_j/n : \quad j = 1, \ldots, n\}$ is dense in $(0, 4)$ giving the result. $\square$

The surface Σ_θ is illustrated in Figure 1.

Theorem 4. *Define $\tilde{a}_i, l_i : \mathbb{R}^3 \backslash \Sigma_\theta \to \mathbb{C}$ for $i = 1, 2, 3$ as the pointwise limits,*

$$\tilde{a}_i(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\,\hbar\to 0\\ n\hbar=\lambda}} \frac{\tilde{A}_i\psi_{n,\theta}(\boldsymbol{x})}{\psi_{n,\theta}(\boldsymbol{x})}, \qquad l_i(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\,\hbar\to 0\\ n\hbar=\lambda}} \frac{L_i\psi_{n,\theta}(\boldsymbol{x})}{\psi_{n,\theta}(\boldsymbol{x})}. \tag{28}$$

Then, for all $\boldsymbol{x} \in \mathbb{R}^3 \setminus \Sigma_\theta$,

$$l_3\cos\theta + \tilde{a}_1\sin\theta = \lambda, \tag{29}$$

$$l_1 \cos\theta + i l_2 - \tilde{a}_3 \sin\theta = 0, \tag{30}$$

$$\tilde{a}_3 \cos\theta + l_1 \sin\theta = 0, \tag{31}$$

$$\tilde{a}_1 \cos\theta + i\tilde{a}_2 - l_3 \sin\theta = 0. \tag{32}$$

Proof. The existence of the limits and the equations (29) - (32) follow from Theorem 3 provided $\psi_{n,\theta}(\boldsymbol{x}) \neq 0$. □

4 The semiclassical Kepler/Coulomb problem

In previous papers [3, 4] we have investigated the semiclassical limit of the atomic elliptic state by considering directly the correspondence limit of $\boldsymbol{Z}^{n,\theta}$ where $\boldsymbol{Z}^{n,\theta}(\boldsymbol{x}) = -i\hbar\nabla \ln \psi_{n,\theta}(\boldsymbol{x})$ and $\psi_{n,\theta}$ is as in equation (27). This limit can be explicitly computed but leads to complicated expressions for $\boldsymbol{Z}$ and the semiclassical Nelson drift field $\boldsymbol{b}$. We now consider this problem from a different perspective by considering the identities in Theorem 4 together with the properties of the underlying classical system.

4.1 Semiclassical mechanics

For $\boldsymbol{x} \in \mathbb{R}^3 \setminus \Sigma_\theta$ we define $\boldsymbol{Z}^{n,\theta}(\boldsymbol{x}) = -i\hbar\nabla \ln \psi_{n,\theta}(\boldsymbol{x})$ which satisfies,

$$E_n = -\frac{\hbar}{2}\nabla \cdot \boldsymbol{Z}^{n,\theta} + \frac{1}{2}|\boldsymbol{Z}^{n,\theta}|^2 - \frac{\mu}{|\boldsymbol{x}|},$$

and we define its semiclassical limit (pointwise limit),

$$\boldsymbol{Z}(\boldsymbol{x}) := \lim_{\substack{n\to\infty,\, \hbar\to 0\\ n\hbar=\lambda}} \boldsymbol{Z}^{n,\theta}(\boldsymbol{x}).$$

If we can determine the vector $\boldsymbol{Z}$ then we have determined (up to a constant) the semiclassical quantum state $\psi_{\text{s.c.}}$ and hence the drift of the associated semiclassical Nelson diffusion process $\boldsymbol{b} = \operatorname{Im}\boldsymbol{Z} - \operatorname{Re}\boldsymbol{Z}$. Assuming that the limit $\boldsymbol{Z}$ exists we must demand that $\boldsymbol{Z}$ satisfies,

$$\frac{1}{2}|\boldsymbol{Z}|^2 - \frac{\mu}{|\boldsymbol{x}|} = -\frac{\mu^2}{2\lambda^2} =: E, \qquad \nabla \wedge \boldsymbol{Z} = 0. \tag{33}$$

Indeed it can be easily verified that $\boldsymbol{Z}$ as defined in (8) has these properties.

We introduce the trajectory $\boldsymbol{X}^0(t)$ defined as the solution for the differential equation,

$$\dot{\boldsymbol{X}}^0(t) = \boldsymbol{b}(\boldsymbol{X}^0(t)), \qquad \dot{\boldsymbol{X}}^0(0) = \boldsymbol{b}(\boldsymbol{x}_0), \qquad \boldsymbol{X}^0(0) = \boldsymbol{x}_0,$$

where we assume that $\boldsymbol{Z}$ is suitably well behaved that $\boldsymbol{X}^0(t)$ exists for $t \in [0, T]$ for some (possibly infinite) $T > 0$. This corresponds to the formal deterministic limit ($\epsilon \to 0$) of the semiclassical Nelson diffusion $\boldsymbol{X}^\epsilon$ as defined in (10).

Theorem 5. *Suppose that (33) holds and that $\dot{\boldsymbol{X}}^0(t)$ is well defined for all $t \in [0, T]$ for some $T > 0$. Then,*

$$\ddot{\boldsymbol{X}}^0(t) = -\nabla \left(-\frac{\mu}{|\boldsymbol{X}^0(t)|} - |\mathrm{Im}\, \boldsymbol{Z}(\boldsymbol{X}^0(t))|^2 \right).$$

Proof. Since $\boldsymbol{b}$ is a gradient it follows that $\ddot{\boldsymbol{X}}^0(t) = -\nabla \left(-2^{-1}|\boldsymbol{b}|^2\right)$ which gives the result. □

Thus we can view $\boldsymbol{X}_t^0$ as the trajectory of a semiclassical particle acted on by a Coulomb potential with a quantum effect given by the potential $-|\mathrm{Im}\, \boldsymbol{Z}|^2$. Indeed it follows from (33) that $\boldsymbol{b}$ can be written in the form,

$$\boldsymbol{b} = \nabla \mathcal{S}$$

for some function $\mathcal{S} = \mathcal{S}(\boldsymbol{x})$ and $\mathcal{S}$ will satisfy the stationary Hamilton-Jacobi equation,

$$\frac{1}{2}|\nabla \mathcal{S}|^2 - \frac{\mu}{|\boldsymbol{x}|} - |\mathrm{Im}\, \boldsymbol{Z}(\boldsymbol{x})|^2 = \frac{-\mu^2}{2\lambda^2}.$$

Thus the drift field $\boldsymbol{b}$ is a perturbation of the velocity field for a Coulomb potential, but it is no longer necessarily even a central force so we cannot expect either the angular momentum $\boldsymbol{l}'$ or the Hamilton-Lenz-Runge vector $\boldsymbol{a}'$ to be constants of the motion. This dynamical system has been extensively examined in [3, 4] but the identities (29) - (32) and the underlying structure they reveal are new.

In fact we actually have two dynamical systems. We can define a second classical mechanical system this time with a complex trajectory $\boldsymbol{\xi}(t)$ defined as the solution for the differential equation,

$$\dot{\boldsymbol{\xi}}(t) = \boldsymbol{Z}(\boldsymbol{\xi}(t)), \qquad \dot{\boldsymbol{\xi}}(0) = \boldsymbol{Z}(\boldsymbol{x}_0), \qquad \boldsymbol{\xi}(0) = \boldsymbol{x}_0,$$

where we assume that $\boldsymbol{Z}$ is suitably well behaved that $\boldsymbol{\xi}(t)$ exists for $t \in [0, \tau]$ for some (possibly infinite) $\tau > 0$.

Theorem 6. *Suppose that (33) holds and that $\dot{\boldsymbol{\xi}}(t)$ is well defined for all $t \in [0, \tau]$ for some $\tau > 0$. Then,*

$$\ddot{\boldsymbol{\xi}}(t) = -\nabla \left(-\frac{\mu}{|\boldsymbol{\xi}(t)|} \right).$$

Proof. Follows as for Theorem 5. □

We note here that $|\boldsymbol{\xi}(t)|$ is not the absolute value of the complex number $\boldsymbol{\xi}(t)$ but is defined by,

$$|\boldsymbol{\xi}(t)|^2 = \xi_1(t)^2 + \xi_2(t)^2 + \xi_3(t)^2$$

where $\boldsymbol{\xi}(t) = (\xi_1(t), \xi_2(t), \xi_3(t)) \in \mathbb{C}^3$.

Thus we can also view $\boldsymbol{Z}$ as defining the velocity field for a classical Coulomb potential but acting on a complex phase space under the constraint that the energy must be real. It follows again that we can find a complex valued function $\mathcal{S}$ which satisfies the Hamilton-Jacobi equation,

$$\frac{1}{2}|\nabla \mathcal{S}|^2 - \frac{\mu}{|\boldsymbol{x}|} = \frac{-\mu^2}{2\lambda^2}.$$

We now look at how Theorem 4 can illuminate the semiclassical mechanics.

4.2 The Semiclassical Identities

Consider the equations (29) - (32) which hold for the semiclassical limit of the atomic elliptic state with eccentricity $e = \sin\theta$. To allow us to consider these equations in the positive and zero energy case we unscale the Hamilton-Lenz-Runge vector by defining,

$$a_i(\boldsymbol{x}) = \sqrt{-2E}\,\tilde{a}_i(\boldsymbol{x}) = \frac{\mu}{\lambda}\tilde{a}_i(\boldsymbol{x}),$$

giving,

$$\frac{\mu}{\lambda} l_3 \cos\theta + a_1 \sin\theta = \mu, \tag{34}$$

$$\frac{\mu}{\lambda} l_1 \cos\theta + i\frac{\mu}{\lambda} l_2 - a_3 \sin\theta = 0, \tag{35}$$

$$a_3 \cos\theta + \frac{\mu}{\lambda} l_1 \sin\theta = 0, \tag{36}$$

$$a_1 \cos\theta + i a_2 - \frac{\mu}{\lambda} l_3 \sin\theta = 0, \tag{37}$$

Table 1: Summary of semiclassical equations.

Parameters	Conic & Group	Identities	Energy Equation
$e = 0$	Circle $SO(4)$	$a_1 + ia_2 = 0$ $l_1 + il_2 = 0$ $l_3 = \lambda$ $a_3 = 0$	$\frac{1}{2}\lvert\boldsymbol{Z}\rvert^2 - \frac{\mu}{\lvert\boldsymbol{x}\rvert} = -\frac{\mu^2}{2\lambda^2}$
$0 < e < 1$, $0 < \lambda < \infty$	Ellipse $SO(4)$	$a_1 + ia_2\sqrt{1-e^2} = \mu e$ $l_1 + il_2\sqrt{1-e^2} = 0$ $\frac{\mu}{\lambda}l_3 - ia_2 e = \mu\sqrt{1-e^2}$ $a_3 - i\frac{\mu}{\lambda}l_2 e = 0$	$\frac{1}{2}\lvert\boldsymbol{Z}\rvert^2 - \frac{\mu}{\lvert\boldsymbol{x}\rvert} = -\frac{\mu^2}{2\lambda^2}$
$e = 1$, $\lambda = \infty$	Parabola $ISO(3)$	$a_1 = \mu$ $l_1 = 0$ $a_2 = 0$ $a_3 = 0$	$\frac{1}{2}\lvert\boldsymbol{Z}\rvert^2 - \frac{\mu}{\lvert\boldsymbol{x}\rvert} = 0$
$e > 1$ $\lambda \mapsto i\lambda$	Hyperbola $SO(3,1)$	$a_1 + a_2\sqrt{e^2-1} = \mu e$ $l_1 + l_2\sqrt{e^2-1} = 0$ $\frac{\mu}{\lambda}l_3 + a_2 e = -\mu\sqrt{e^2-1}$ $a_3 - \frac{\mu}{\lambda}l_2 e = 0$	$\frac{1}{2}\lvert\boldsymbol{Z}\rvert^2 - \frac{\mu}{\lvert\boldsymbol{x}\rvert} = \frac{\mu^2}{2\lambda^2}$

which hold for the elliptical case.

By writing the eccentricity as e where $e = \sin\theta$ we can then extend these equations to include the circular/elliptic, parabolic and hyperbolic cases subject to suitable substitutions for λ corresponding to negative, zero and positive energy E respectively. These four cases are listed in Table 1 giving the equations (34) - (37) (in a rearranged form) together with the 'energy' equation (33) in each case.

A simple calculation working from the definition (28) gives,

$$\boldsymbol{l} = \boldsymbol{x} \wedge \boldsymbol{Z}, \qquad \boldsymbol{a} = \boldsymbol{Z} \wedge (\boldsymbol{x} \wedge \boldsymbol{Z}) - \frac{\mu \boldsymbol{x}}{|\boldsymbol{x}|}, \tag{38}$$

and so the equations in Table 1 can be viewed as polynomial equations for the components of $\boldsymbol{Z}$.

Suppose that we take the equations in Table 1 as defining the vector field $\boldsymbol{Z}$. We have the following result:-

Theorem 7. *The equations listed in Table 1 have:-*

1. *in the circular case, a unique solution (which is complex) given by,*

$$\boldsymbol{Z} = \boldsymbol{Z}^C := \frac{i\mu}{\lambda}\frac{\boldsymbol{x}}{|\boldsymbol{x}|} + \frac{\mu}{\lambda}\frac{\lambda^2}{\mu(x_1 + ix_2)}\left(-i, 1, 0\right).$$

2. *in the elliptic case, two solutions (both complex) one of which is given by,*

$$\boldsymbol{Z} = \boldsymbol{Z}^E := \frac{i\mu}{\lambda}\frac{\left(1+\gamma^E\right)}{2}\frac{\boldsymbol{x}}{|\boldsymbol{x}|} + \frac{\mu}{\lambda}\frac{\left(\gamma^E - 1\right)}{2e}(-i, \sqrt{1-e^2}, 0),$$

where,

$$\gamma^E = \sqrt{1 - \frac{4}{\nu^E}}, \qquad \nu^E(\boldsymbol{x}) = \frac{\mu}{\lambda^2}\left(|\boldsymbol{x}| - \frac{x_1}{e} - i\frac{x_2}{e}\sqrt{1-e^2}\right).$$

3. *in the parabolic case, two solutions (both real) given by,*

$$\boldsymbol{Z} = \boldsymbol{Z}^{P\pm} := \pm\sqrt{\mu}\frac{\operatorname{sgn}(x_2)}{\sqrt{|\boldsymbol{x}| - x_1}}\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \pm \sqrt{\mu}\frac{\operatorname{sgn}(x_2)}{\sqrt{|\boldsymbol{x}| - x_1}}\left(-1, 0, 0\right).$$

4. *in the hyperbolic case, two solutions (both real) one of which is given by,*

$$\boldsymbol{Z} = \boldsymbol{Z}^H := \frac{\mu}{\lambda}\frac{\left(1+\gamma^H\right)}{2}\frac{\boldsymbol{x}}{|\boldsymbol{x}|} + \frac{\mu}{\lambda}\frac{\left(\gamma^H - 1\right)}{2e}(-1, \sqrt{e^2-1}, 0),$$

where,

$$\begin{aligned} \gamma^H \quad &= \operatorname{sgn}\left(x_2 + x_1\sqrt{e^2-1}\right)\sqrt{1 - \tfrac{4}{\nu^H}}, \\ \nu^H(\boldsymbol{x}) \quad &= -\tfrac{\mu}{\lambda^2}\left(|\boldsymbol{x}| - \tfrac{x_1}{e} + \tfrac{x_2}{e}\sqrt{e^2-1}\right). \end{aligned}$$

Proof. Noting that each l_i is linear in the components of $\boldsymbol{Z}$ it it possible to eliminate two of the Z_is between the five equations in each case. This reduces the problem to:-

1. (circular case) a pair of quadratic equations which have a single common root,

(ii)-(iv) (other cases) a cubic and quartic equation which have a pair of common roots.

Identifying these common roots gives the result. □

The root $\boldsymbol{Z}^E$ corresponds to the known solution given in (8) and $\boldsymbol{Z}^H$ corresponds to the natural extension of this solution to the hyperbolic case. It is important to note that we are free to choose the two sgn terms in the parabolic and hyperbolic cases. For instance showing that $\boldsymbol{Z}^H$ is a solution in the hyperbolic case relies only on the fact that $(\gamma^H)^2 = 1 - \frac{4}{\nu^H}$. The choices made here are natural in the sense that with this choice in the parabolic case,

$$\boldsymbol{Z}^{P+} = \lim_{\substack{\lambda\to\infty, e\to 1\\ \Lambda=\frac{\lambda^2}{\mu}(1-e^2)}} \boldsymbol{Z}^E,$$

where the semi-latus rectum Λ is held fixed and the complex square root in the definition of γ^E is taken as in [3]. These choices will be discussed in more detail later. We do not give an explicit expression for the second solution in the hyperbolic/elliptic cases due to restrictions of space. They can easily be calculated by factoring out the given root from the polynomials. The semiclassical Nelson drift field $\boldsymbol{b}$ for each $\boldsymbol{Z}$ is shown in Figure 2 in the plane $z = 0$.

Before we move on to a detailed discussion of the dynamical systems defined by these vectors, we highlight that we can also find the semiclassical wave functions corresponding to these values of $\boldsymbol{Z}$:-

Theorem 8. *The vectors $\boldsymbol{Z}^{(\star)}$ correspond to the following semiclassical wave functions in the sense that $\boldsymbol{Z}^{(\star)} = -i\hbar\nabla \ln \psi^{(\star)}$:-*

$$\psi^C = (x_1 + ix_2)^{\lambda/\hbar} \exp\left(-\tfrac{\mu}{\lambda\hbar}|\boldsymbol{x}|\right),$$

$$\psi^E = \nu^E(\boldsymbol{x})^{\lambda/\hbar}(1+\gamma^E(\boldsymbol{x}))^{2\lambda/\hbar} \exp\left(-\tfrac{\mu}{\lambda\hbar}|\boldsymbol{x}| + \tfrac{\lambda}{2\hbar}(1-\gamma^E(\boldsymbol{x}))\nu^E(\boldsymbol{x})\right),$$

$$\psi^P = \exp\left(i\tfrac{2\sqrt{\mu}}{\hbar}\,\mathrm{sgn}\,(x_2)\sqrt{|\boldsymbol{x}| - x_1}\right),$$

$$\psi^H = \nu^H(\boldsymbol{x})^{i\lambda/\hbar}(1+\gamma^H(\boldsymbol{x}))^{2i\lambda/\hbar} \exp\left(-\frac{\mu}{i\lambda\hbar}|\boldsymbol{x}| + \frac{i\lambda}{2\hbar}(1-\gamma^H(\boldsymbol{x}))\nu^H(\boldsymbol{x})\right).$$

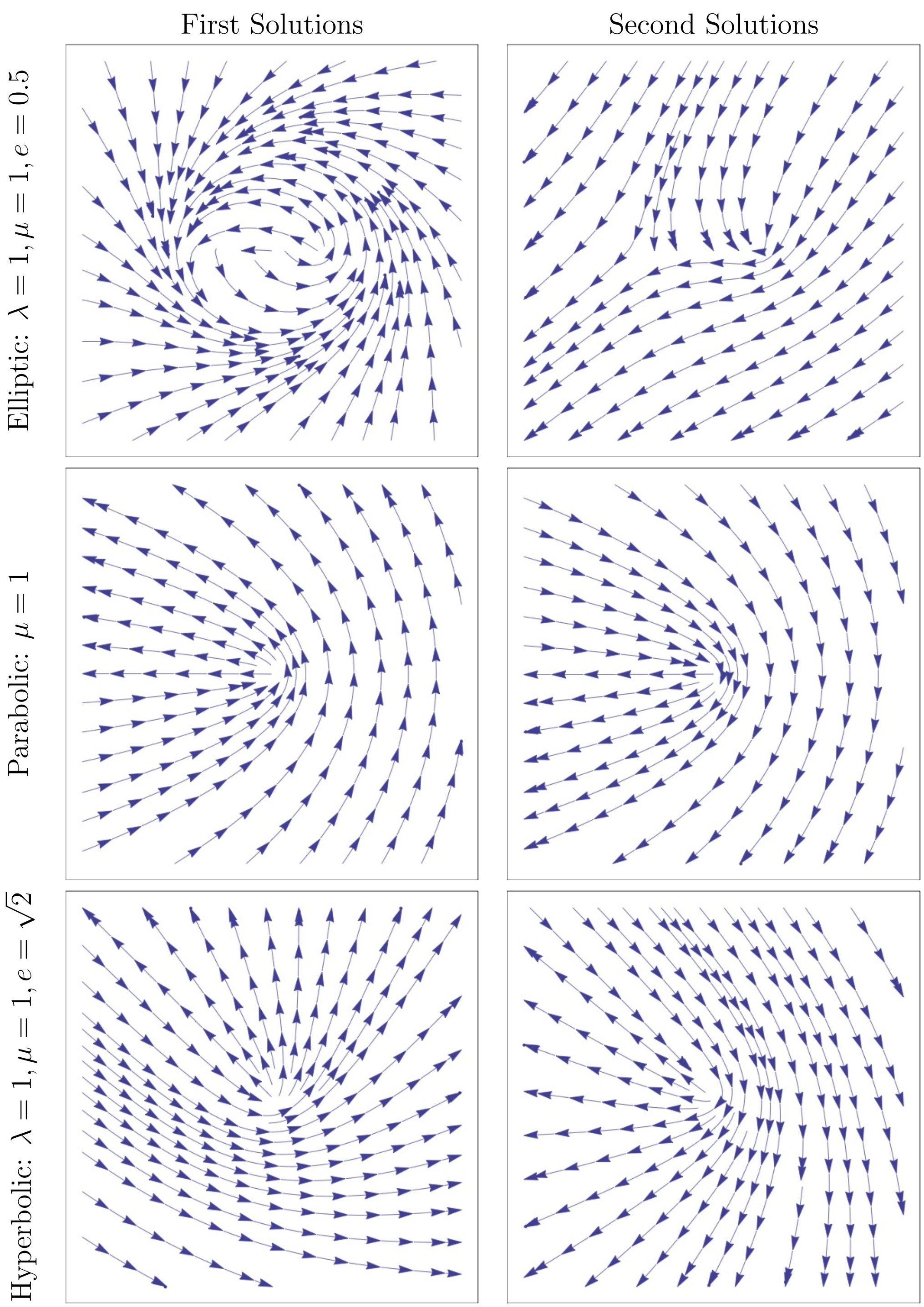


Figure 2: The drift fields $\boldsymbol{b}$ in the elliptic, parabolic and hyperbolic cases in the plane $x_3 = 0$.

4.3 Discussion

We have identified semiclassical quantities $\boldsymbol{a} = (a_1, a_2, a_3)$ and $\boldsymbol{l} = (l_1, l_2, l_3)$ which are complex valued functions of the variables $\boldsymbol{x}$ and $\boldsymbol{Z}$ satisfying the equations listed in Table 1. These quantities are the semiclassical analogues to the Hamilton-Lenz-Runge vector $\boldsymbol{a}'$ and the angular momentum $\boldsymbol{l}'$ which are the constants of the classical motion. We have then used the identities contained in Table 1 to find complex valued vector fields $\boldsymbol{Z} = \boldsymbol{Z}(\boldsymbol{x})$ for which there are 9 possible solutions (1 circular, 2 each elliptical, parabolic and hyperbolic), four of which are listed in Theorem 7. These vector fields $\boldsymbol{Z}(\boldsymbol{x})$ can be used to determine two classical mechanical systems $\boldsymbol{X}^0(t)$ (the deterministic limit of the semiclassical Nelson diffusion) and $\boldsymbol{\xi}(t)$ (a complex valued solution to the Coulomb/Kepler problem) where,

$$\dot{\boldsymbol{X}}^0(t) = \boldsymbol{b}(\boldsymbol{X}^0(t)), \qquad \dot{\boldsymbol{\xi}}(t) = \boldsymbol{Z}(\boldsymbol{\xi}(t)),$$

and $\boldsymbol{b}(\boldsymbol{x}) = \operatorname{Re} \boldsymbol{Z}(\boldsymbol{x}) - \operatorname{Im} \boldsymbol{Z}(\boldsymbol{x})$.

Firstly let us consider the system given by $\boldsymbol{\xi}(t)$. It follows from Theorem 6 that this system is simply the classical mechanics governed by the Hamiltonian,

$$H(\boldsymbol{x}, \boldsymbol{Z}) = \frac{|\boldsymbol{Z}|^2}{2} - \frac{\mu}{|\boldsymbol{x}|},$$

on the phase space $\mathbb{C}^6$ with coordinates $(\boldsymbol{x}, \boldsymbol{Z})$ where $|\boldsymbol{x}|^2 = x_1^2 + x_2^2 + x_3^2$. We note that the energy equation in Table 1 imposes the constraint in each case that the energy is real valued for the path $\boldsymbol{\xi}(t)$. Indeed the path $\boldsymbol{\xi}(t)$ is such that the vectors $\boldsymbol{a}$ and $\boldsymbol{l}$ will be complex valued constants corresponding to the Lenz-Runge vector and angular momentum. Moreover, we can define the natural Poisson bracket,

$$\{f, g\} = \sum_{j=1}^{3} \left(\frac{\partial f}{\partial x_i} \frac{\partial g}{\partial Z_j} - \frac{\partial g}{\partial x_i} \frac{\partial f}{\partial Z_j} \right),$$

and it follows immediately that $\boldsymbol{a}$ and $\boldsymbol{l}$ are then generators of $SO(4)$, $ISO(3)$ or $SO(3,1)$ depending on the case considered.

If we instead consider the system $\boldsymbol{X}^0(t)$ then it follows from Theorem 5 that we have a real valued classical mechanical system governed by the Hamiltonian,

$$H(\boldsymbol{x}, \boldsymbol{p}) = \frac{|\boldsymbol{p}|^2}{2} - \frac{\mu}{|\boldsymbol{x}|} - |\operatorname{Im} \boldsymbol{Z}(\boldsymbol{x})|^2,$$

on the phase space $\mathbb{R}^6$ with coordinates $(\boldsymbol{x}, \boldsymbol{p})$. As we noted previously, if the vector field $\boldsymbol{Z}(\boldsymbol{x})$ is non-real for $\boldsymbol{x} \in \mathbb{R}^3$ then this system is no longer even a central force. The angular monentum and Lenz-Runge vector are therefore not constants of the motion but instead the equations in Table 1 hold.

It is interesting to note that $\boldsymbol{Z}^{P\pm}$ and $\boldsymbol{Z}^{H}$ are real valued for all $\boldsymbol{x} \in \mathbb{R}^3$. It follows that the corresponding drift fields coincide:

$$\boldsymbol{b}^{P\pm} = \boldsymbol{Z}^{P\pm}, \qquad \boldsymbol{b}^{H} = \boldsymbol{Z}^{H}.$$

Thus we can conclude from Theorems 5 and 6 that in the parabolic and hyperbolic cases that our two dynamical systems $\boldsymbol{X}^0(t)$ and $\boldsymbol{\zeta}(t)$ coincide and give a solution for the classical Coulomb problem. Thus we see that in both parabolic and hyperbolic cases that $\boldsymbol{a}$ and $\boldsymbol{l}$ are constants of the motion determined by the initial conditions with the additional constraint that the equations in Table 1 must hold.

Let us consider in some detail the classical mechanics determined by the vector field $\boldsymbol{b}^{P+} = \boldsymbol{Z}^{P+}$. We know that the solution to the initial value problem,

$$\dot{\boldsymbol{X}}^0(t) = \boldsymbol{b}^{P+}(\boldsymbol{X}^0(t)), \qquad \dot{\boldsymbol{X}}^0(0) = \boldsymbol{b}^{P+}(\boldsymbol{x}_0), \qquad \boldsymbol{X}^0(0) = \boldsymbol{x}_0,$$

corresponds to the classical mechanics for the Coulomb potential with zero energy and so all trajectories are parabolas contained in the plane,

$$x_3 = \left(\frac{x_{0,3}}{x_{0,2}}\right) x_2, \qquad \boldsymbol{x}_0 = (x_{0,1}, x_{0,2}, x_{0,3}),$$

with semimajor axis coinciding with the x_1 axis, focus at the origin and semilatus rectum $\frac{|\boldsymbol{l}|^2}{\mu} = \frac{l_2^2+l_3^2}{\mu}$.

However the field $\boldsymbol{Z}^{P+}$ is singular not just at the origin but also across the positive x_1 axis where $|\boldsymbol{x}| - x_1 = 0$. Indeed as our equations in Table 1 determining the field $\boldsymbol{Z}^{P+}$ are a limit of the elliptical equations it follows from Lemma 2 that they cannot be expected to hold in the plane $x_2 = 0$. However this can be overcome by using the constants of the motion. A simple calculation gives the drift field along a fixed trajectory as,

$$\boldsymbol{Z}^{P+} = \left(\frac{\sqrt{|\boldsymbol{x}| - x_1}\,\operatorname{sgn}(x_2)}{|\boldsymbol{x}|}, \frac{l_3}{|\boldsymbol{x}|}, -\frac{l_2}{|\boldsymbol{x}|}\right). \tag{39}$$

The appropriate value of $\boldsymbol{Z}^{P+}$ across the positive x_1 axis is thus determined by the initial condition which fixes the values of l_2 and l_3. Clearly the trajectories of the classical system are focussed into the positive x_1 axis forming a caustic as shown in Figure 3 (a).

The role of the sgn function in the definition of $\boldsymbol{Z}^{P\pm}$ can now be seen by considering the vector field,

$$\tilde{\boldsymbol{Z}}^{P+} := \sqrt{\mu}\frac{1}{\sqrt{|\boldsymbol{x}| - x_1}}\frac{\boldsymbol{x}}{|\boldsymbol{x}|} + \sqrt{\mu}\frac{1}{\sqrt{|\boldsymbol{x}| - x_1}}\,(-1, 0, 0)\,.$$

For this field every trajectory is directed towards the positive x_1 axis where they terminate (in the first parabolic solution shown in Figure 2 the arrows in the upper half plane are reversed; in Figure 3 all trajectories move towards the caustic). This forms a caustic for the corresponding Hamilton-Jacobi equation,

$$\frac{1}{2}|\nabla\mathcal{S}|^2 - \frac{\mu}{|\boldsymbol{x}|} = 0,$$

with solution $\mathcal{S} = \tilde{\mathcal{S}}^{P+}$ where from Theorem 8,

$$\tilde{\mathcal{S}}^{P+}(\boldsymbol{x}) = 2\sqrt{\mu}\sqrt{|\boldsymbol{x}| - x_1}, \qquad \tilde{\boldsymbol{Z}}^{P+} = \nabla\tilde{\mathcal{S}}^{P+}(\boldsymbol{x}).$$

Clearly the solution $\mathcal{S} = \tilde{\mathcal{S}}^{P+}$ is differentiable except on the positive x_1 axis where $|\boldsymbol{x}| - x_1 = 0$. Alternatively the solution $\mathcal{S} = \mathcal{S}^{P+}$ defined by,

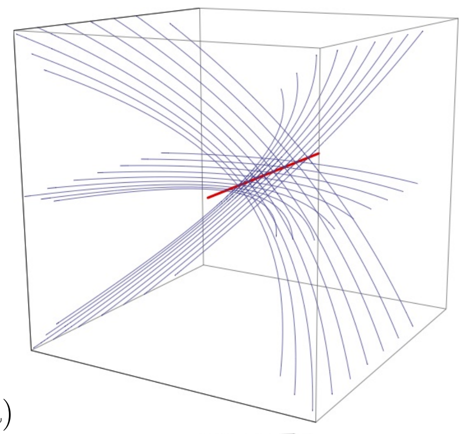
$$\mathcal{S}^{P+}(\boldsymbol{x}) = 2\sqrt{\mu}\,\mathrm{sgn}\,(x_2)\sqrt{|\boldsymbol{x}| - x_1}, \qquad \boldsymbol{Z}^{P+} = \nabla\mathcal{S}^{P+}(\boldsymbol{x}),$$

when restricted to one of the classical planes of motion given by $x_3 = (x_{0,3}/x_{0,2})x_2$, is C^1 across the positive x_1 axis with the corresponding trajectories passing through the caustic however now $\mathcal{S}^{P+}$ is discontinuous across the rest of the surface $x_2 = 0$ (see Figure 4). Thus we see that our choice of sgn functions in the definition of $\boldsymbol{Z}^{P\pm}$ corresponds to a choice of boundary conditions for the Hamilton-Jacobi equation across the caustic. Indeed, we can calculate the derivatives on the positive x_1 axis explicitly to give,

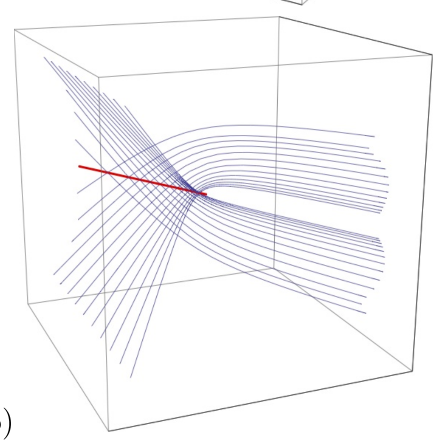
$$\frac{\partial}{\partial x_2}\mathcal{S}^{P+}(x_1, x_2, (x_{0,3}/x_{0,2})x_2)\bigg|_{x_2=0} = \sqrt{2}\sqrt{\frac{1}{x_1}\left(1 + \left(\frac{x_{0,3}}{x_{0,2}}\right)^2\right)}.$$

We note that it follows from (39) that any parabola crosses the positive x_1 axis at the point,

$$x_1 = \frac{(l_3x_{0,2} - l_2x_{0,3})^2}{2(x_{0,2}^2 + x_{0,3}^2)}.$$

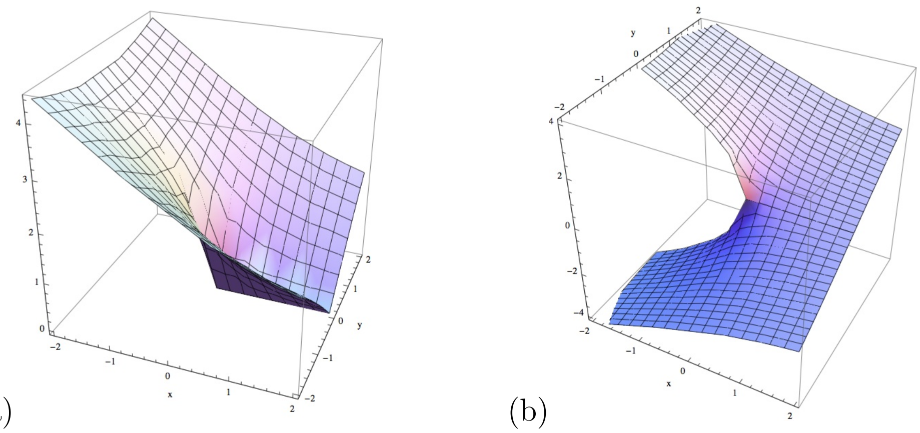


(a)



(b)

Figure 3: Some trajectories for the classical dynamical systems in (a) the parabolic case ($\mu = 1$) and (b) the hyperbolic case ($\mu = 1$, $\lambda = 1$ and $e = 2$) with the caustic highlighted (red).



(a) (b)

Figure 4: The functions (a) $\tilde{\mathcal{S}}^{P+}$ and (b) $\mathcal{S}^{P+}$ with $\mu = 1$ plotted in the plane $z = 0$ showing the caustic in (a) and its smoothing in (b).

A similar analysis holds for the hyperbolic case. The system now corresponds to solutions to the classical Coulomb problem with positive energy so all trajectories are hyperbolas contained in the plane,

$$x_3 = \left(\frac{x_{0,3}}{x_{0,2} + x_{0,1}\sqrt{e^2-1}}\right)\left(x_2 + x_1\sqrt{e^2-1}\right), \qquad \boldsymbol{x}_0 = (x_{0,1}, x_{0,2}, x_{0,3}),$$

with eccentricity $\frac{|\boldsymbol{a}|}{\mu} = \frac{\sqrt{\left(e^2 l_2^2 + \lambda^2 + l_3^2\right)}}{\lambda}$, semilatus rectum $\frac{|\boldsymbol{l}^2|}{\mu} = \frac{e^2 l_2^2 + l_3^2}{\mu}$ and semi-major axis λ^2/μ with focus at the origin whose axis is given by,

$$\frac{1}{e\sqrt{e^2 l_2^2 + \lambda^2 + l_3^2}}\left(\lambda - l_3\sqrt{e^2-1}, -\lambda\sqrt{e^2-1} - l_3, e^2 l_2\right).$$

Again we note that the field $\boldsymbol{Z}^H$ is not defined everywhere, here the caustic being given by the line,

$$\nu^H = 0 \qquad \Leftrightarrow \qquad x_3 = 0, \quad x_2 + x_1\sqrt{e^2-1} = 0, \quad x_1 > 0.$$

This problem can again be overcome by utilising the constants of the motion to rewrite $\boldsymbol{Z}^H$ along a fixed trajectory as,

$$\begin{aligned}\boldsymbol{Z}^H \quad &= \Big(-\tfrac{a_2\lambda|\boldsymbol{x}| + e\sqrt{e^2-1}\lambda l_2^2 + \sqrt{e^2-1}l_2 x_3 + \lambda x_2}{\lambda l_3|\boldsymbol{x}|}, \\ &\qquad \tfrac{a_1\lambda|\boldsymbol{x}| - e\lambda l_2^2 - l_2 x_3 + \lambda x_1}{\lambda l_3|\boldsymbol{x}|}, -\tfrac{e\lambda l_2 + x_3}{\lambda|\boldsymbol{x}|}\Big).\end{aligned}$$

Thus we see that $\boldsymbol{Z}^H$ assumes values on the caustic determined by the initial condition. This again explains the sgn term in $\boldsymbol{Z}^H$ which allows the trajectories to pass through the caustic shown in Figure 3 (b). Again the function $\mathcal{S} = \mathcal{S}^H$ where,

$$\mathcal{S}^H(\boldsymbol{x}) := \lambda \ln|\nu^H(\boldsymbol{x})| + 2\lambda \ln|1 + \gamma^H(\boldsymbol{x})| + \frac{\mu}{\lambda}|\boldsymbol{x}| + \frac{\lambda}{2}(1 - \gamma^H(\boldsymbol{x}))\nu^H(\boldsymbol{x})$$

and $\boldsymbol{Z}^H = \nabla \mathcal{S}^H$ is the solution to our Hamilton Jacobi equation with appropriate boundary condition across the caustic.

For the circular and elliptic cases our vector fields $\boldsymbol{Z}^C$ and $\boldsymbol{Z}^E$ are complex valued and so the two dynamical systems $\boldsymbol{X}^0(t)$ and $\boldsymbol{\zeta}(t)$ are distinct. Indeed $\boldsymbol{Z}^C$ and $\boldsymbol{Z}^E$ are only real valued on the corresponding Kepler circle/ellipse thus we have Keplerian motion on the classical orbits corresponding to the correct energy and given eccentricity.

It is also interesting that there is no obvious physical significance to the second solution in the elliptical case for the Nelson diffusion system.

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