SEMICLASSICAL (STOCHASTIC) QUANTUM MECHANICS

Piotr Garbaczewski(1)

Institute of Theoretical Physics, University of Wrocław, PL-50-205 Wrocław, Poland

Dariusz Prorok(2)

Mathematics Department King's College, Strand, London, United Kingdom

Summary:

We explore the probabilistic aspects of the quantized Coulomb-Kepler problem in the (extremally) semiclassical regime.

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(1) Delivered by P.G.

(2) On leave from the ITP, University of Wrocław

1. Statement of purpose: Departing from the stochastic mechanics model for the condensation of planets out of a protosolar nebula one arrives at the Schrödinger equation for the central problem. To explain how elliptic Kepler trajectories arise in this setting, we investigate the semiclassical regime of appropriate wave packets. The stochastic mechanics motivations follow from [1-3,34-36,28,29], while the relevant semiclassical analysis is related to [4-33].

2. Paradigm case, the Coulomb-Kepler problem and Gaussians.

The Coulomb-Kepler problem both in its classical and quantum versions is a standard text-book companion of the harmonic oscillator in any descriptiom of basic physical concepts. It is a part of folk-lore that everything relevant has been said and nothing relevant can be added to the issue. The situation is however not that obvious.

As is well known[20] the Wilson-Sommerfeld quantization rule, in case of the Coulomb-Kepler problem incorporates contributions from both circular and elliptic orbits (although the circular orbits suffice for the understanding of the spectrum). It is however somehow overlooked that Schrödinger's claim "wave groups can be constructed which move around highly quantized Kepler ellipses and are the representation by wave mechanics of the hydrogen electron", until recently has not received an adequate attention. This gap in the understanding of the fundamental model was the reason of a renaissance in the study of semiclassical features of the quantum Coulomb-Kepler problem[21-34].

Our own interest in the subject can be motivated as follows:

(i) Nelson's stochastic mechanics links the time development of quantum states with this for the appropriate stochastic (diffusion) processes. A better understanding of the physical meaning of this stochasticity should be arrived at while passing

to the semiclassical regime. The analysis of the issue is far from being complete, apart from the numerical study of[2,3]. Recently the correspondence limit of the sample path of Nelson's mechanics for the $\psi_{n,n-1,n-1}$ orbital was shown[34] to converge in the L^2 sense to a classical trajectory (circular Kepler orbit). There is a close relationship of this investigation with our own[28-30] search for elliptic Kepler orbits in the framework of stochastic mechanics.
From another standpoint[32,33] the classical limits of quantal probability distributions ($\hbar \to 0$ at constant energy) were studied and the corresponding classical ensembles introduced. In particular classical orbits for a statistical beam undergoing classical Coulomb scattering were derived in this way, see also[31].

(ii) The stochastic model for the orbits of planets and satellites[35,36,34] is based on the Schrödinger type equation for the central problem. Being in principle capable of providing the segregation of matter mechanisms, with respect to the implementation of realistic classical motions, it could be linked with the circular orbit prediction of[22] only.
However, <u>one must be able to explain how stochastic mechanics leads to the coplanar elliptic orbits, consistent with Kepler's third law of planetary motion.</u>
The discussion of the circular case can be found in[34] with the qualitative argument that the accretion of matter by the diffusing planetesimal makes the diffusion coefficient $\varepsilon^2=\hbar/m(t)$ to diminish with the growth of time. As a consequence the Nelson diffusion should converge to a Keplerian orbit.

(iii) Since Gaussian wave packets are particularly useful for the study of semiclassical features of the quantum motion (6-11,22,26-30), see also[37,38], we get confronted with the problem of how to reconcile the classical time development of coherent state labels

$$\dot{\alpha} = \{\alpha, H_c\} \qquad \dot{\bar{\alpha}} = \{\bar{\alpha}, H_c\}. \tag{2.1}$$

with the time dependence of coherent states. In general[6]

$$|\alpha,t) = \exp(-\frac{i}{\hbar} Ht)|\alpha) \neq |\alpha(t))$$
$$H_{cl} = (\alpha|:H:|\alpha) \tag{2.2}$$

where $\alpha(t)$ is determined by (2.1).
This problem we encountered before[28-30] but it is implicit as well in[27]
The comparison of the time evolution of coherent states to this a classical particle would have in the same potential, has been the subject of analytic estimates ($\hbar \to 0$ regime) in[7,10] while a numerical analysis of the issue was attempted in[38] in slightly different context. Since generally the coherent states of interest fail to obey the exact Schrödinger equation, the main goal of the recent paper[30] was to investigate the accuracy with which they can be viewed to <u>approximate</u> true solutions. Since we refer to the central problem, let us mention that we use the Gaussian states, although the $|x| \to 0$ singularity would apparently lead to difficulties. We are motivated by the semiclassical analysis of[21,22], and we account for the fact that the semi-

classical wave must be concentrated around a classical trajectory, which never crosses the origin. It is a reasonable working assumption to exclude the ball of the size of the nucleus surrounding the singularity of the potential from considerations.

In the next section, motivated by[30] we shall discuss this approximation in more detail. Albeit disregarding the spreading effects (which may be significant in the narrow tube along the Kepler orbit[22]) we find the approximation satisfactory in the proper parameter regime (mass and minimal distance from the central body, while on the orbit). We emphasize at this point that a mathematical correctness of the standard $\hbar \to 0$ prescription not always is physically clear : it is inevitable to identify proper physical quantities, with numerical values sufficiently large compared to $\hbar$ (which is kept fixed as a universal constant) to arrive at a physically sound picture.

The parameter implementing the semiclassical regime in below will not be $\hbar$ but the (large) mass parameter. In case of realistic masses spreading effects do not matter on time scales equating the age of the Universe .

3. Non-spreading ("frozen") coherent states as approximate solutions of the Schrödinger equation in case of the Coulomb-Kepler problem

Inserting the wave function

$$\psi(\vec{x},t) = \phi(\vec{x},t) \exp \frac{i}{\hbar} S(\vec{x},t) \tag{3.1}$$

to the equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left(- \frac{\hbar^2}{2m} \Delta + V(\vec{x}) \right)\psi \tag{3.2}$$

we arrive at:

$$\left[\frac{\partial S}{\partial t} + H(\frac{\partial S}{\partial x_i}, x_i, t)\right]\phi + (-i\hbar)\left[\frac{\partial \phi}{\partial t} + \frac{1}{m}\nabla S \nabla \phi + \frac{1}{2m}\phi \Delta S\right] - \frac{\hbar}{2m}\Delta\phi = 0 \tag{3.3}$$

Let us investigate what would have happen if we choose:

$$\phi(\vec{x},t) = (2\pi\sigma)^{-3/4} \exp\left[-\frac{1}{4\sigma}(\vec{x} - \vec{Q}(t))^2\right]$$

$$S(\vec{x},t) = S_o + \vec{P}(t)\cdot(\vec{x} - \vec{Q}(t) + \\ + \int_0^t \{\vec{P}(\tau)\dot{\vec{Q}}(\tau) - H(\vec{P}(\tau),\vec{Q}(\tau))\}d\tau - \frac{3}{2}\hbar\omega t \tag{3.4}$$

where $\vec{Q}(t)$, $\vec{P}(t)$ are classical solutions of Hamilton equations generated by the Hamiltonian

$$H(\vec{Q},\vec{P}) = \frac{1}{2m}\vec{P}^2 + V(\vec{Q}) \tag{3.5}$$

We denote $\vec{Q}(t=0)=\vec{Q}_o$, $\vec{P}(t=0)=\vec{P}_o$.

(3.4) implies that:

$$\frac{\partial \phi}{\partial t} = \frac{1}{2\sigma}(\vec{x} - \vec{Q})\cdot\dot{\vec{Q}}\phi$$

$$\frac{\partial \phi}{\partial x_i} = -\frac{1}{2\sigma}(x_i - Q_i)\phi \tag{3.6}$$

$$\frac{\partial S}{\partial x_i} = P_i \qquad \frac{\partial^2 S}{\partial x_i^2} = 0$$

and because of $\dot{Q}_i = \frac{\partial H}{\partial P_i} = \frac{1}{m}P_i$ there holds:

$$\frac{\partial \phi}{\partial t} + \frac{1}{m}\nabla S \cdot\nabla\phi + \frac{1}{2m}\phi\Delta S = 0 \tag{3.7}$$

Therefore the imaginary part of (3.3) disappears.
Taking into account the formula:

$$\frac{\partial S}{\partial t} = \dot{\vec{P}}(\vec{x} - \vec{Q}) - \vec{P}\dot{\vec{Q}} + \vec{P}\dot{\vec{Q}} - H(\vec{P},\vec{Q},t) - \frac{3}{2}h\omega =$$

$$= \dot{\vec{P}}(\vec{x} - \vec{Q}) - H(\vec{P},\vec{Q},t) - \frac{3}{2}h\omega \qquad (3.8)$$

$$H\left(\frac{\partial S}{\partial x},x,t\right) = H(\vec{P},\vec{Q} + (\vec{x}-\vec{Q}),t) =$$

$$= H(\vec{P},\vec{Q},t) - \dot{\vec{P}}(\vec{x}-\vec{Q}) + O((\vec{x}-\vec{Q})^2)$$

where

$$O((\vec{x}-\vec{Q})^2) = V(\vec{x}) - V(\vec{Q}) - \sum_{i=1}^{3}\frac{\partial V(Q)}{\partial Q_i}(x_i-Q_i) =$$

$$= \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2 V(Q)}{\partial Q_i \partial Q_j}(x_i-Q_i)(x_j-Q_j) + \qquad (3.9)$$

$$+ \frac{1}{3!}\sum_{i,j,k=1}^{3}\frac{\partial^3 V(Q)}{\partial Q_i \partial Q_j \partial Q_k}(x_i-Q_i)(x_j-Q_j)(x_k-Q_k) +$$

$$+ \dots$$

while

$$\Delta\phi = \frac{1}{2\sigma}\left(\frac{1}{2\sigma}(\vec{x} - \vec{Q})^2 - 3\right)\phi(\vec{x},t) \qquad (3.10)$$

we find that the left-hand-side of (3.3) produces the term

$$L(\vec{x},t) = \left[O((\vec{x}-\vec{Q})^2) - \frac{m\omega^2}{2}(\vec{x} - \vec{Q})^2\right]\phi(\vec{x},t) \qquad (3.11)$$

which is the measure of inaccuracy with which $\psi(\vec{x},t)$ solves the

Schrödinger equation.

Let us investigate the case of the central potential $V(x) = -\frac{A}{|\vec{x}|}$ where $A=Ze^2$ in case of Coulomb problem, while $A = \gamma mM$ for the Kepler case.

For all $|\vec{x}| \geq a > 0$, a finite it is easy to verify that:

$$O((\vec{x} - \vec{Q})^2) = -\frac{A}{x}\frac{1}{Q^3}\left[x\vec{Q}(\vec{x} - \vec{Q}) - (x - Q)Q^2\right] \tag{3.12}$$

$$x = |\vec{x}| \qquad Q = |\vec{Q}|$$

Consequently (3.11) reads:

$$L(\vec{x},t) = -(2\pi\sigma)^{-3/4}\left\{\frac{A}{x}\frac{1}{Q^3}\left[x\vec{Q}(\vec{x}-\vec{Q}) - (x-Q)Q^2\right] + \frac{1}{2}m\omega^2(\vec{x}-\vec{Q})^2\right\}\exp\left[-\frac{1}{4\sigma}(\vec{x} - \vec{Q})^2\right] \tag{3.13}$$

Our inaccuracy estimate will pertain to the semiclassical regime. For say $|\vec{x}-\vec{Q}| \leq 0{,}1\, Q$ we have:

$$(\vec{x} - \vec{Q})^2 = x^2 + Q^2 - 2Qx\cos(\vec{x},\vec{Q}) \cong$$
$$\cong x^2 + Q^2 - 2Qx = (x - Q)^2 \tag{3.14}$$

so that:

$$L(\vec{x},t) \cong -(2\pi\sigma)^{-3/4}\left[\frac{A}{x}\frac{1}{Q^2}(x - Q)^2 + \frac{1}{2}m\omega^2(x - Q)^2\right]\cdot \exp\left[-\frac{1}{4\sigma}(x - Q)^2\right] \tag{3.15}$$

Because the maximum of the function $(x-Q)^2 \exp\left[-\frac{1}{4\sigma}(x-Q)^2\right]$ at its points $x_{1,2}=Q\pm 2\sqrt{\sigma}$ equals $4\sigma e^{-1}$, upon $\sqrt{\sigma}<<Q$ we can write $x_{1,2} \cong Q$. Furthermore if $|x-Q| \cong 0{,}1\ Q$ then there holds

$$- L(\vec{x},t) \leq (2\pi\sigma)^{-3/4} \left(\frac{A}{x}\, 10^{-2} + \frac{1}{2} m\omega^2 Q^2 10^{-2} \right) \exp\left(-\frac{1}{4} Q^2 10^{-2} \right) \tag{3.16}$$

We are interested in the semiclassical features of the system, hence admitting Q to be of the macroscopic size we realize that (3.16) is very small (the exponential damping). Denoting $x=x_{1,2}$ we arrive at:

$$- L(\vec{x}_{1,2},t) \cong (2\pi\sigma)^{-3/4} \left(\frac{A}{Q^3} + \frac{1}{2} m\omega \right)^2 4\sigma e^{-1} =$$

$$= 4(2\pi)^{-3/4}\, e^{-1} \sigma^{1/4} \left(\frac{A}{Q^3} + \frac{1}{2} m\omega^2 \right) \tag{3.17}$$

The frequency ω is a free parameter, which can be appropriately adjusted. Minimizing (3.17) with respect to ω and accounting for $\sigma=\hbar/2m\omega$ we find:

$$\begin{aligned} u(\omega) &= \frac{A}{Q^3}\, \omega^{-1/4} + \frac{1}{2} m\omega \\ u'(\omega) &= \frac{1}{4}\, \omega^{3/4} \left(-\frac{A}{Q^3}\, \omega^{-2} + \frac{7}{2} m \right) = 0 \\ u''(\omega) &= \frac{5}{16}\, \omega^{-9/4} \frac{A}{Q^3} + \frac{21}{32} m\, \omega^{-1/4} \geq 0 \end{aligned} \tag{3.18}$$

the minimum being reached at $\omega = (\frac{A}{m})^{1/2} Q^{-3/2}$ when

$$- L(\vec{x}_{1,2},t) = \left(\frac{\hbar}{m}\right)^{1/4}\left[\frac{A}{Q^3}\left(\frac{A}{m}\right)^{-1/2} Q^{3/8} + \right. \tag{3.19}$$

$$\left. + \frac{1}{2}m\left(\frac{A}{m}\right)^{7/8} Q^{-21/8}\right] \cong \hbar^{1/4}m^{-1/8}A^{7/8}Q^{-21/8}$$

Hence

$$|L(\vec{x},t)| \leq h^{1/4}\ m^{-1/8}\ A^{7/8}\ Q^{-21/8} \tag{3.20}$$

If we consider $|x-Q|>>4\sigma$, then $L(\vec{x},t)$ is negligibly small in virtue of the damping factor $\exp\left[-\frac{1}{4\sigma}(x-Q)^2\right]$ n the above estimate ω depends on time through the classical trajectory $Q(t)$. To be a proper (time independent) frequency parameter it needs a proper fit of Q_{min} (we equate it to the major semi-axis of the ellipse)instead of $Q(t)$. Then $\omega = \left(\frac{A}{m}\right)^{1/2} Q_{min}^{-3/2}$,and the Kepler period for motions on elliptic orbits does arise. Now:

$$|L(\vec{x},t)| \leq \hbar^{1/4}\ m^{-1/8}\ A^{7/8}\ Q_{min}^{-21/8} \tag{3.21}$$

$$A_{Coul} = Ze^2 \qquad\qquad A_{Kepl} = \gamma mM$$

After accounting for the exponential term, we realize that our inaccuracy measure makes essential contributions in a close surrounding of the classical trajectory. It is amusing to observe that the estimate (3.21) gives account of the three regimes exploited in the study of the semiclassical features of the hydrogen problem. Namely the $\hbar^{1/4}$ factor refers to the $\hbar \to 0$ regime, the $m^{-1/8}$ factor refers to the $m \to \infty$ case, while $Q_{min}^{-21/8}$ factor is related to the $l,n \to \infty$ regime studied in[21,22].

Both in the Coulomb and Kepler case the combined effect of m large, Q_{min} large (while keeping the very small $\hbar$ fixed), is capable of giving rise to essentially classical features of the quantum motion.

Let us emphasize that apart from the discussed inaccuracy measure, it is the width of the wave packet $2\sqrt{2\sigma}$ which is a proper measure of how classical the quantum motion is.

Let us examine the meaning of our estimates for the realistic examples of the electrostatic and gravitational potentials. In case of the hydrogen atom, for the choice of the classical orbit (Rydberg atoms) $Q(t) \geqq 10^{-2}$m there holds

$$|L(\vec{x},t)| \leqq 10^{-24}[J/m^{3/2}] , \qquad \omega = 10^4[s^{-1}] \tag{3.22}$$

while the wave packet width in each of the coordinates

$$\Delta x_i = 2\sqrt{2\sigma} = 2 \cdot 10^{-4}[m] \tag{3.23}$$

proves that on a short time scale only (see e.g. at[22] for the analysis of spreading times, while at[24] for the description of Rydberg atoms and their life-times) the semiclassical picture is reliable.

Notice that the gravitational motion of the Earth around the Sun corresponds to the Gaussian with

$$|L(\vec{x},t)| \leq 2\cdot 10^{-2}[J/m^{3/4}] , \qquad \omega = 10^{-6}[s^{-1}] \tag{3.24}$$

where however:

$$\Delta x_i = 2\sqrt{2\sigma} \cong 10^{-26}[m] \tag{3.25}$$

to be compared with (3.23).

Consequently we are capable of constructing approximate solutions of the Schrödinger equation, which display basic features of the classical motion of the mass point representing the Earth around the point-like Sun.

The corresponding coherent state certainly does not reflect any realistic triggering (fluctuations) of the Earth trajectory, but rather an extremely narrow tube of nearby classical orbits.

Notice that the characterization of the pure Coulomb case

$$|L(\vec{x},t)| \le \hbar^{1/4}\ m^{-1/2}\ A^{7/8}\ Q_{min}^{-21/8}$$

$$\sqrt{2\sigma} = \left(\frac{\hbar}{m\omega}\right)^{1/2} = h^{1/2}\ m^{-1/4}\ A^{-1/4}\ Q_{min}^{3/4}\quad ,\ A = Ze^2 \tag{3.26}$$

is different from this of the pure Kepler problem:

$$|L(\vec{x},t)| \le \hbar^{1/2}\ m^{3/4}(\gamma M)^{7/8}\ Q_{min}^{-21/8}$$

$$\sqrt{2\sigma} = \hbar^{1/2}\ m^{-1/2}(\gamma M)^{-1/4}\ Q_{min}^{3/4} \tag{3.27}$$

It is amusing to observe a striking correlation between m and Q_{min} for planets of the solar system which is reflected by the numerical values of the upper bound for $|L(\vec{x},t)|$ and the width $2\sqrt{2\sigma}$.

These values read respectively:

Mercury	$\lvert L(\vec{x},t)\rvert \le 2\ 10^{-2}$	$\sqrt{2\sigma}$ =	$2,2\ 10^{-26}$
Venus	$4,5\ 10^{-2}$		10^{-26}
Earth	$1,7\ 10^{-2}$		10^{-26}
Mars	10^{-3}		$4.3\ 10^{-26}$

Jupiter	$\lvert L(x,t)\rvert \leq$ 1,7 10^{-2}		1,9 10^{-27}
Saturn	1,44 10^{-3}		0,56 10^{-26}
Uranus	5,7 10^{-5}		2,4 10^{-26}
Neptune	2 10^{-5}		3 10^{-26}
Pluto	4,8 10^{-7}		4,7 10^{-27}

Even in this extremal regime we still deal with Gaussians, and Nelson's approach induces sample paths of the (classically controlled)Wiener noise.Albeit mathematically acceptable , this picture does not seem to be physically correct;it was the planetary dust which was the reason of randomness in the time evolution of the planetesimal. The accretion of matter cannot last indefinitely, since there is a finite amount of dust accessible. Moreover, with the time passing,the no-where differentiable sample trajectories should be in principle replaced by piecewise differentiable with a finite number of random disturbances in a finite time interval , which get eventually transformed into everywhere differentiable ones,when there is practically no dust around the planet.

This problem needs further investigations, see also [41].
Would it amount to the jump process approximation of the diffusion process ?

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