FACTA UNIVERSITATIS
Series: **Physics, Chemistry and Technology** Vol. 15, N° 2, 2017, pp. 71 - 79
https://doi.org/10.2298/FUPCT1702071P

THE FIRST AND SECOND MOMENTS FOR THE QUANTUM BROWNIAN PLANAR ROTATOR IN EXTERNAL HARMONIC CLASSICAL FIELD†

UDC 53.072 : 539.194

Igor Petrović[1], Jasmina Jeknić-Dugić[2*]

[1]Sokobanja, Serbia
[2]Department of Physics, Faculty of Sciences and Mathematics, University of Niš, Niš, Serbia

Abstract. *We derive explicit expressions for the first and second moments as well as the correlation function for a planar (one-dimensional) quantum Brownian rotator placed in the external harmonic potential. Our results directly provide the standard deviations for the azimuthal angle and the canonically conjugate angular momentum for the rotator. We find that there are some significant physical differences between this model and the free rotator model, which is well investigated in the literature.*

Key words: *open quantum systems, quantum Brownian motion, quantum rotator.*

1. INTRODUCTION

The theory of open quantum systems has a very important role in many applications of quantum physics since perfect isolation of quantum systems is not possible in practice (Breuer and Petruccione 2002, Rivas and Huelga 2011). Quantum Brownian motion (QBM, Caldeira and Leggett 1983) is paradigmatic for the field of open quantum systems theory (Breuer and Petruccione 2002). Description of quantum decoherence (Giulini et al 1996, Dugić 2004) as well as modeling of "quantum dissipation" is directly provided for QBM as a realistic physical situation with the well-defined classical counterpart. The usefulness of the QBM model places the model at the heart of applications regarding the nano- and mesoscopic systems and some artificial setups as well as regarding the related emerging technologies, e.g. (Milburn 1987, Jones 2008, Kottas et al 2005).

Received: January 15th, 2017; accepted: December, 21st, 2017.
† This research is partially financially supported by the Ministry of Education, Science and Technological Development, Republic of Serbia, Grant 171028.
* **Corresponding author**: Jasmina Jeknić-Dugić
Department of Physics, Faculty of Science and Mathematics, Višegradska 3, 18000 Niš, Serbia
E-mail: jjeknic@pmf.ni.ac.rs

The standard model of Brownian motion (Caldeira and Legett 1983, Breuer and Petruccione 2002) regards a point-like particle with the mass m and is directly applicable (mathematically isomorphic) to an arbitrary set of the particle's degrees of freedom. From the basic quantum master equation, the so-called Caldeira-Leggett equation (Caldeira and Leggett 1983), the *general* form of the differential equations can be deduced straightforwardly for the first and second moments of the basic observables - of the position and momentum observables. In the Caldeira-Leggett model the bath is a collection of harmonic oscillators and the coupling to the reduced system is linear and weak (Caldeira and Legett 1983, Breuer and Petruccione 2002). The simplest and most detailed studied case is free Brownian motion. A somewhat complicated and even more relevant case is the case of a Brownian particle in the external harmonic field (Caldeira and Legett 1983, Breuer and Petruccione 2002). We are not aware of any explicit results presented in the literature regarding the aforementioned first and second moments for a Brownian particle in the external harmonic field.

In this paper we go even beyond the standard (Caldeira and Legett 1983, Breuer and Petruccione 2002) translational Brownian motion. Bearing in mind the importance of the molecular nano-cogwheels for the emerging nano-technology, we employ the quantum-mechanical model for the classical Brownian-*rotator*-model of the molecular cogwheels (Kottas et al 2005, Browne and Feringa 2006, Hutchinson et al 2014, Korobenko et al 2014, etc.) with the "azimuthal" angle $\varphi \in [0,2\pi]$ as the only degree of freedom and the moment of inertia denoted I. The importance of the harmonic potential for the quantum *rotational* Brownian motion here considered stems from at least the following two sources. First, in realistic physical situations, the rotating parts of the molecular rotors may rest on the solid surfaces, where the links with the surfaces (actually the chemical bonds) provide an effective torsional field for rotation (Kottas et al 2005). The first approximation for such situations is a harmonic field for small angles of rotation. Similarly, external electric fields exerted on polar molecules often lead to an effective harmonic field (Kottas et al 2005) as it is assumed in our considerations. Second, numerical studies, e.g. (Boyke Schönborn et al 2009), of the effective external potential for molecular rotations point out to the existence of the local minima for rotation. Again, for small rotations (used as the boundary condition for the model), in the vicinity of the bottom of a local minimum, the dominant dynamics are harmonic-oscillation rotations around the equilibrium position, which is defined as the bottom of the potential well.

In comparison with the results for the free rotator out of any external field, we can conclude that there are some significant physical differences between these two models that are subject of brief discussion in Section 5. Clearly, the results of this paper equally regard the translational model.

2. THE TASK

The original Caldeira-Leggett model of QBM (Caldeira and Leggett 1983) regards a one-dimensional particle with a single position (Descartes) degree of freedom, x, and mass m. The conjugate momentum operator p satisfies the commutator equation $[x,p] = i\square/2\pi \equiv i\hbar$, where h is the Planck constant. Transition to the rotational model of the Caldeira-Leggett master equation as presented in (Suzuki and Tanimura 2001) is justified by the analogous commutator relation $[\varphi, L_z] = i\hbar$, where there now appear the rotational variables φ and L_z, instead of the Descartes x and p, while the moment of inertia of the rotator, denoted I, exchanges the mass m of the translational model. While we adopt the model proposed in (Suzuki and Tanimura 2001) without a modification, the following remark is in order.

As distinct from the continuous and unbounded x and p, the angle variable φ is bounded (its eigenvalues $\varphi \in [0,2\pi]$), while L_z is with the pure discrete spectrum ($m\hbar, m = 0, \pm 1, \pm 2, \dots$). Then the commutation relation $[\varphi, L_z] = i\hbar$ cannot be given an analogous interpretation as the commutator $[x,p] = i\hbar$ (Jordan 1927, Breitenberger 1985, Deck and Ozturk 1994). Rather, the analogy between the translational Descartes and the rotational observables is limited to the small values of the standard deviation $\Delta\varphi$ (Breitenberger 1985). Together with the assumption of the small rotations emphasized in Introduction, this limitation constitutes the basis of our considerations in the rest of this paper.

Bearing this in mind, as well as the model proposed in (Suzuki and Tanimura 2001), in analogy with the equations (3.426)-(3.430) in (Breuer and Petruccione 2002), it directly follows for the planar rotator in external field, $V(\varphi)$, the differential equations for the first and the second moments, as well as the correlation function for the φ and L_z observables:

$$\frac{d\langle\varphi(t)\rangle}{dt} = \frac{1}{I} L_z(t), \tag{1}$$

$$\frac{d\langle L_z(t)\rangle}{dt} = -\langle V'(\varphi(t))\rangle - 2\gamma\langle L_z(t)\rangle, \tag{2}$$

$$\frac{d\langle\varphi^2(t)\rangle}{dt} = \frac{1}{I}\langle L_z(t)\varphi(t) + \varphi(t)L_z(t)\rangle, \tag{3}$$

$$\frac{d\langle L_z(t)\varphi(t)+\varphi(t)L_z(t)\rangle}{dt} = -2\langle\varphi(t)V'(\varphi(t))\rangle - 2\gamma\langle L_z(t)\varphi(t) + \varphi(t)L_z(t)\rangle + \frac{2}{I}\langle L_z^2(t)\rangle, \tag{4}$$

$$\frac{d\langle L_z^2(t)\rangle}{dt} = -\langle L_z(t)V'(\varphi(t)) + V'(\varphi(t))L_z(t)\rangle - 4\gamma\langle L_z^2(t)\rangle + 4I\gamma kT. \tag{5}$$

The symbol "$\langle A\rangle = trA\rho$" is the mean (average value) of the A observable for the system in the state ρ (which for $t > 0$ is always a mixed state represented by a "statistical operator", i.e. by a "density matrix", $\rho^2 \neq \rho$). The constant γ is the so-called "damping rate" originating from the influence of the environment with an Ohmic spectral density, at high temperature T and k is the Boltzmann constant. The "I" stands for the moment of inertia of the rotator. The prime in the subscript of the potential observable, $V(\varphi)$, denotes the derivation over φ: $V'(\varphi) \equiv dV(\varphi)/d\varphi$. For simplicity, we further assume the time dependence of the observables without explicit writing.

Hence for the harmonic potential with the circular frequency ω,

$$V(\varphi) = \frac{1}{2}I\omega^2\varphi^2, \tag{6}$$

the equations (1)-(5) take the following form:

$$\frac{d\langle\varphi\rangle}{dt} = \frac{1}{I} L_z, \tag{7}$$

$$\frac{d\langle L_z\rangle}{dt} = -I\omega^2\langle\varphi\rangle - 2\gamma\langle L_z\rangle, \tag{8}$$

$$\frac{d\langle\varphi^2\rangle}{dt} = \frac{1}{I}\langle L_z\varphi + \varphi L_z\rangle, \tag{9}$$

$$\frac{d\langle L_z\varphi+\varphi L_z\rangle}{dt} = -2I\omega^2\langle\varphi^2\rangle - 2\gamma\langle L_z\varphi + \varphi L_z\rangle + \frac{2}{I}\langle L_z^2\rangle, \tag{10}$$

$$\frac{d\langle L_z^2\rangle}{dt} = -I\omega^2\langle L_z\varphi + \varphi L_z\rangle - 4\gamma\langle L_z^2\rangle + 4I\gamma kT. \tag{11}$$

Our objective is to accurately solve these equations and calculate the standard deviations, as well as the correlation function for φ and L_z. The application of the solutions to be presented below is constrained by the assumptions underlying the derivation of the Caldeira-Leggett equation that reads (Caldeira and Leggett 1983, Breuer and Petruccione 2002):

$$\frac{kT}{\hbar\omega} > 1 \text{ (high-temperature limit)} \tag{12}$$

$$\omega \gg \gamma \text{ (weak interaction with the environment).} \tag{13}$$

3. SOLUTIONS OF THE EQUATIONS

It is easy to obtain solutions to the equations (7) and (8) from which it directly follows:

$$\langle\varphi(t)\rangle^2 = e^{-2\gamma t}\left(\langle\varphi(0)\rangle^2 cos^2\omega t + \frac{\langle L_z(0)\rangle^2}{I^2\omega^2} sin^2\omega t + \frac{\langle\varphi(0)\rangle\langle L_z(0)\rangle}{I\omega} sin2\omega t\right), \tag{14}$$

$$2\langle\varphi(t)\rangle\langle L_z(t)\rangle = e^{-2\gamma t}\left(2\langle\varphi(0)\rangle\langle L_z(0)\rangle\ cos2\omega t + \left[\frac{\langle L(0)\rangle^2}{I\omega} - \langle\varphi(0)\rangle^2 I\omega\right] sin2\omega t\right), \tag{15}$$

$$\langle L_z(t)\rangle^2 = e^{-2\gamma t}(\langle L_z(0)\rangle^2 cos^2\omega t + I^2\omega^2\langle\varphi(0)\rangle^2 sin^2\omega t - \langle\varphi(0)\rangle\langle L_z(0)\rangle I\omega sin2\omega t). \tag{16}$$

On the other hand, the equations (9)-(11) represent a set of coupled, first-order non-homogeneous linear differential equations. Here we apply the standard matrix method of solving such a set of differential equations (Nagle et al 2011).

With a change in notation, $x(t) \equiv \langle\varphi^2(t)\rangle, y(t) \equiv \langle L_z(t)\varphi(t) + \varphi(t)L_z(t)\rangle \equiv \langle L_z\varphi + \varphi L_z\rangle_t, z(t) \equiv \langle L_z^2(t)\rangle, D \equiv 4I\gamma kT$, we introduce the matrices (again, for simplicity, omitting the time dependence in what follows)

$$X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{17}$$

$$M = \begin{pmatrix} 0 & \frac{1}{I} & 0 \\ -2I\omega^2 & -2\gamma & \frac{2}{I} \\ 0 & -I\omega^2 & -4\gamma \end{pmatrix}, \tag{18}$$

and for the non-homogeneous part:

$$F = \begin{pmatrix} 0 \\ 0 \\ D \end{pmatrix}, \tag{19}$$

so we can write (9)-(11) in the matrix form:

$$\frac{d}{dt}X = MX + F. \tag{20}$$

Solving the eigenvalue problem for the matrix M gives the following eigenvalues

$$\left\{-2\gamma, -2\left(\gamma - \sqrt{-4\omega^2 + \gamma^2}\right), -2\left(\gamma + \sqrt{-4\omega^2 + \gamma^2}\right)\right\},$$

which, with the use of the equation (13), implies the approximate values:

$$\{-2\gamma, -2(\gamma - i\omega), -2(\gamma + i\omega)\}, \tag{21}$$

and the respective (approximate) eigenvectors:

$$\begin{pmatrix} \frac{1}{I^2\omega^2} \\ -\frac{2\gamma}{I\omega^2} \\ 1 \end{pmatrix}, \begin{pmatrix} -\frac{\omega^2-2i\gamma c}{I^2\omega^4} \\ -\frac{2(\gamma+i\omega)}{I\omega^2} \\ 1 \end{pmatrix}, \begin{pmatrix} -\frac{\omega^2+2ib\omega}{I^2\omega^4} \\ -\frac{2(\gamma-i\omega)}{I\omega^2} \\ 1 \end{pmatrix}. \tag{22}$$

From the equations (21)-(22), a particular solution, $N(t)$, due to the nonhomogeneous part is obtained by solving the matrix equation:

$$\begin{pmatrix} \frac{e^{-2\gamma t}}{I^2\omega^2} & -\frac{\left(-2i\gamma\omega+c^2\right)e^{-2(\gamma-i)t}}{I^2\omega^4} & -\frac{\left(2i\gamma\omega+c^2\right)e^{-2(\gamma+i)t}}{I^2\omega^4} \\ -\frac{2\gamma e^{-2\gamma t}}{I\omega^2} & -\frac{2(\gamma+i\omega)e^{-2(\gamma-i\omega)t}}{I\omega^2} & -\frac{2(\gamma-i\omega)e^{-2(\gamma+i\omega)t}}{I\omega^2} \\ e^{-2\gamma t} & e^{-2(\gamma-i\omega)t} & e^{-2(\gamma+i\omega)t} \end{pmatrix} N(t) = F. \tag{23}$$

After integration of the solutions over time t, the result reads:

$$Y(t) = \int N(t)dt = \begin{pmatrix} \frac{De^{2\gamma t}}{4\gamma} \\ \frac{(2i\gamma+\omega)De^{2(\gamma-i\omega)t}}{8(\gamma-i\omega)\omega} \\ \frac{(-2i\gamma+\omega)De^{2(\gamma+i\omega)t}}{8(\gamma+i\omega)\omega} \end{pmatrix}. \tag{24}$$

Hence the general solutions can be presented as:

$$x(t) = \left(A + \frac{De^{2\gamma t}}{4\gamma}\right)\frac{e^{-2\gamma t}}{I^2\omega^2} - \left(B + \frac{(2i\gamma+c)De^{2(\gamma-i\omega)t}}{8(\gamma-i\omega)\omega}\right)\frac{(-2i\gamma\omega+c^2)e^{-2(\gamma-i\omega)t}}{I^2\omega^4} - \left(C + \frac{(-2i\gamma+\omega)De^{2(\gamma+ic)t}}{8(\gamma+i\omega)\omega}\right)\frac{(2i\gamma\omega+\omega^2)e^{-2(\gamma+i\omega)t}}{I^2\omega^4}, \tag{25}$$

$$y(t) = -\left(A + \frac{De^{2\gamma t}}{4\gamma}\right)\frac{2\gamma e^{-2\gamma t}}{I\omega^2} - \left(B + \frac{(2i\gamma+\omega)De^{2(\gamma-i\omega)t}}{8(\gamma-i\omega)c}\right)\frac{2(\gamma+i\omega)e^{-2(\gamma-i\omega)t}}{I\omega^2} - \left(C + \frac{(-2i\gamma+\omega)De^{2(\gamma+i\omega)t}}{8(\gamma+i\omega)\omega}\right)\frac{2(\gamma-i\omega)e^{-2(\gamma+i\omega)t}}{I\omega^2}, \tag{26}$$

$$z(t) = \left(A + \frac{De^{2\gamma t}}{4\gamma}\right)e^{-2\gamma t} + \left(B + \frac{(2i\gamma+\omega)De^{2(\gamma-i\omega)t}}{8(\gamma-i\omega)\omega}\right)e^{-2(\gamma-i\omega)t} + \left(C + \frac{(-2i\gamma+\omega)De^{2(\gamma+i\omega)t}}{8(\gamma+i\omega)\omega}\right)e^{-2(\gamma+i\omega)t}, \tag{27}$$

with the unknown constants, A, B, C, for the homogeneous part of the equations (9)-(11).

By introducing the initial values, $x \equiv x(t=0), y \equiv y(t=0), z \equiv z(t=0)$, the solutions for the constants A, B, C in the same order of the approximation equation (13), i.e. $\frac{\gamma}{\omega} \to 0$, read:

$$A = -\frac{D}{4\gamma} + \frac{1}{2}I^2\omega^2 x + \frac{I\gamma y}{2} + \frac{z}{2}, \tag{28}$$

$$B = \frac{(\gamma-i\omega)D - 2a^2\omega^4 x - 2(\gamma-i\omega)\omega^2 a y + 2(2i\gamma+\omega)\omega z}{8\omega^2}, \tag{29}$$

$$C = B^{*} = \frac{(\gamma+i\omega)D-2a^2\omega^4x-2(\gamma+i\omega)\omega^2ay+2(-2i\gamma+\omega)\omega z}{8c^2}. \quad (30)$$

After a straightforward but tedious calculation, substitution of the equations (28)-(30) into (22)-(27) and returning the original notation, we obtain the solutions to the equations (9)-(11) with the approximation equation (13), i.e. $\frac{\gamma}{\omega} \to 0$:

$$\langle\varphi^2(\mathrm{t})\rangle = e^{-2\gamma t}\left(-\frac{4I\gamma kT}{4I^2\omega^2}\left(\frac{1}{\gamma}+\frac{1}{\omega^2}(-\gamma\cos 2\omega t+\omega\sin 2\omega t)\right)+\langle\varphi^2(0)\rangle\left(cos^2\omega t+\frac{\gamma}{\omega}\sin 2\omega t\right)+\frac{\langle L_z\varphi+\varphi L_z\rangle_{t=0}}{2I\omega}(2\gamma\, sin^2\omega\mathrm{t}+\omega\sin 2\omega\mathrm{t})+\frac{\langle L_z(0)^2\rangle}{I^2\omega^2}\left(\sin^2\omega\mathrm{t}-2\frac{\gamma^2}{\omega^2}\cos 2\omega\mathrm{t}\right)\right)+\frac{kT}{\mathrm{I}\omega^2}, \quad (31)$$

$$\langle L_z\varphi+\varphi L_z\rangle_t = e^{-2\gamma t}\left(\frac{4\gamma kT}{\omega^2}sin^2\omega t-\langle\varphi^2(0)\rangle(2I\,\gamma\, sin^2\omega t+I\,\omega\sin 2\omega t)+\langle L_z\varphi+\varphi L_z\rangle_{t=0}\left(-\frac{\gamma^2}{\omega^2}\,sin^2\omega t+\cos 2\omega t\right)-\langle {L_z}^2(0)\rangle\left(\frac{2\gamma}{I\omega^2}\sin^2\omega\mathrm{t}-\frac{1}{I\omega}\sin 2\omega\mathrm{t}\right)\right), \quad (32)$$

$$\langle {L_z}^2(t)\rangle = e^{-2\gamma t}\left(\langle L_z(0)^2\rangle\left(cos^2\omega t-\frac{\gamma}{2\omega}\sin 2\omega\mathrm{t}\right)+I^2\omega^2\langle\varphi^2(0)\rangle\, sin^2\omega t+\langle L_z\varphi+\varphi L_z\rangle_{t=0}\left(I\gamma\;\, sin^2\omega t-\frac{I\omega}{2}\sin 2\omega\mathrm{t}\right)+I\gamma kT\left(-\frac{1}{\gamma}+\frac{\gamma}{\omega^2}\cos 2\omega t+\frac{1}{\omega}\sin 2\omega\mathrm{t}\right)\right)+IkT. \quad (33)$$

4. The Standard Deviations and Correlation Function

From the equations (14)-(17) and (31)-(33), we finally obtain the desired standard deviations and the correlation function:

$$\Delta\varphi(t) = \sqrt{\langle\varphi^2(t)\rangle-\langle\varphi(t)\rangle^2} = \sqrt{e^{-2\gamma t}\left(\left(\Delta\varphi(0)\right)^2cos^2\omega t+\frac{\sigma_{L\varphi}(0)}{2I\omega}\sin 2\omega\mathrm{t}+\frac{\left(\Delta L_z(0)\right)^2}{I^2\omega^2}\sin^2\omega\mathrm{t}\right)+\frac{kT}{\mathrm{I}\omega^2}(1-e^{-2\gamma t})+\mathrm{O}\left(\frac{\gamma}{\omega}\right)}, \quad (34)$$

$$\sigma_{L_z\varphi}(t) = \langle L_z\varphi+\varphi L_z\rangle_t-2\langle\varphi(t)\rangle\langle L_z(t)\rangle = e^{-2\gamma t}\left(\frac{4\gamma kT}{\omega^2}sin^2\omega t-I\,\omega\left(\Delta\varphi(0)\right)^2\sin 2\omega t+\sigma_{L\varphi}(0)cos2\omega t-\frac{1}{I\omega}\left(\Delta L_z(0)\right)^2 sin2\omega t\right)+\mathrm{O}\left(\frac{\gamma}{\omega}\right), \quad (35)$$

$$\Delta L_z(t) = \sqrt{\langle {L_z}^2(t)\rangle-\langle L_z(t)\rangle^2} = \sqrt{e^{-2\gamma t}\left(\left(\Delta L_z(0)\right)^2\,cos^2\omega t+I^2\omega^2\left(\Delta\varphi(0)\right)^2\,sin^2\omega t-\frac{I\omega}{2}\sigma_{L\varphi}(0)\sin 2\omega\mathrm{t}\right)+IkT(1-e^{-2\gamma t})+\mathrm{O}\left(\frac{\gamma}{\omega}\right)}. \quad (36)$$

In the asymptotic limit ($t \to \infty$), the equations (34)-(36) give (while neglecting the terms proportional to $\frac{\gamma}{\omega}$):

$$\lim_{t\to\infty} \Delta\varphi(t) = \sqrt{\frac{kT}{I\omega^2}}, \tag{37}$$

$$\lim_{t\to\infty} \sigma_{L\varphi}(t) = 0\,, \tag{38}$$

$$\lim_{t\to\infty} \Delta L_z(t) = \sqrt{IkT}. \tag{39}$$

5. DISCUSSION

Nature's biological motors serve as inspirations for the creation of small-molecule systems that undergo controllable motion. Molecular rotors and propellers are interesting, primarily because of their potential applications in such molecular machines (Kottas et al. 2005). In order to construct a complex molecular machine, a number of building blocks are generally required, and a high degree of controlled relative motion between its parts is essential for the machine to produce the desired operation. By controlling the translational and rotational movements of the components in the machine, coupled with an inflow of external energy, it is possible to obtain the predetermined function. From all the above, it follows that the most important requirement for the successful application of molecular rotors in molecular machines is the controllability of the rotational movement.

When considering molecular machines and their operation, it should be noted that the forces that control the movement of macroscopic objects have little relevance to molecular machines of nano dimensions. For large objects, inertial terms, which depend on the mass of the particle, dominate the motion. As the particle's size decreases to or below the micrometer scale, viscous forces and Brownian motion become dominant while momentum and gravity become increasingly irrelevant (Jones 2008, Breuer and Petruccione 2002, Kottas et al 2005). Molecular rotors are subject to constant influence of Brownian motion (Kottas et al 2005), so it is preferred that they have the maximum possible robustness with respect to it. If all this is taken into account, the conclusion is that it can be very useful to find an expression for the standard deviation of the azimuthal angle and the canonically conjugate angular momentum of the molecular rotor which is under the influence of Brownian motion. This constitutes the main motivation for this paper as briefly emphasized in Introduction.

For a free Brownian rotator out of any external field, the (exact) equation (3.441) in (Breuer and Petruccione 2002) gives in the asymptotic limit:

$$\lim_{t\to\infty} \Delta\varphi(t) = \sqrt{\frac{kT}{I\gamma}t}, \tag{40}$$

$$\lim_{t\to\infty} \sigma_{L\varphi}(t) = \frac{kT}{\gamma}, \tag{41}$$

$$\lim_{t\to\infty} \Delta L_z(t) = \sqrt{IkT}, \tag{42}$$

that concurs with the classical counterpart obtained from the solution of the corresponding Langevin equation (Breuer and Petruccione 2002) for the "position" variable φ.

The equations (37)-(39) are the rotator-system counterpart of the well-known expressions (see the equation (3.424) in (Breuer and Petruccione 2002)) for the point-like Brownian particle in the external harmonic potential. While the equation (3.424) follows from an approximate treatment of the Caldeira-Leggett master equation, our expressions (37)-(39) follow from the exact equations (1)-(5). A comparison of the equations (40)-(42) with the equations (37)-(39) clearly distinguishes the following physically substantial distinctions between the two models. First, there is no time dependence in the equation (37), thus emphasizing the *existence of the stationary state*, which does not exist for the free Brownian particle - see the equation (40). Second, for the angle-observable we obtain significantly smaller values due to the equation (13). This can be seen by re-writing the equation (37) as:

$$\lim_{t\to\infty} \Delta\varphi(t) = \sqrt{\frac{kT}{\mathrm{I}\omega^2}} = \sqrt{\frac{kT}{\mathrm{I}\gamma}t}\ \sqrt{\frac{1}{\omega t}\frac{\gamma}{\omega}}\ , \tag{43}$$

with the distinguished small terms and time independence of $\Delta\varphi(t)$.

Finally, the product of the standard deviations

$$\lim_{t\to\infty} \Delta\varphi(t)\,\Delta L_z(t) = \frac{kT}{\omega} > \frac{\hbar}{2}, \tag{44}$$

where the last inequality follows from the equation (12). The equation (44) suggests that the stationary (asymptotically time-independent) state of the harmonic Brownian rotator is not of the minimal uncertainty, however revealing the possibility to assume that the final state is of the Gaussian form—compare to Section 3.6.2.2 in (Breuer and Petruccione 2002). These are important conclusions regarding the dynamics of the considered systems that can be used in some practical applications, for example in modeling a molecule as a rotator or as a gear like system, as key elements in natural and artificial molecular machines. (Kottas et al 2005, Browne and Feringa 2006, Hutchinson et al 2014, Korobenko et al 2014). Our results directly extend towards investigating dynamical stability depending on the rotator's geometrical size and shape for realistic physical and chemical situations. To this end, the ongoing research results will be presented elsewhere.

6. Conclusion

Our results provide explicit mathematical forms for the standard deviations for the azimuthal angle and the canonically conjugate angular momentum of a planar (one-dimensional) quantum Brownian rotator placed in the external harmonic potential. In comparison with the well-known free Brownian rotator, we observe the existence of the stationary state in the asymptotic limit ($t \to \infty$), as well as significantly smaller standard deviations and the correlation-function for the rotator exerted to the external harmonic potential. The consequences of our findings for realistic physical and chemical situations will be presented in the sequel.

References

Boyke Schönborn, J., Rainer Herges, J., Hartke, B., 2009. J. Chem. Phys. **130**, 234906
Breitenberger, E., 1985. Found. Phys. **15,** 353
Breuer, H.-P., Petruccione, F., 2002. The Theory of Open Quantum Systems, Clarendon Press, Oxford.
Browne, W., Feringa, B.L., 2006. Nature Nanotech. **1**, 25-35
Caldeira A.O., Leggett A.J., 1983 Physica.A **121**, 587-616
Deck,. R. T., Ozturk, N., 1994. Found. Phys. Lett. **7,** 419

Dugić, M., 2004, Decoherence in the classical limit of quantum mechanics, SFIN XVII(2), Institute of Physics, Belgrade (in Serbian)

Giulini D., Joos E., Kiefer C., Kupsch J., Stamatescu I.-O., Zeh H. D., 1996, Decoherence and the Appearance of a Classical World in Quantum Theory, Springer, Berlin

Hutchison J.A., et al, 2014, Nature Nanotech. 9, 131–136

Jones, R.A., 2008, Soft Machines: Nanotechnology and Life, Oxford University Press

Jordan, P., 1927. Z. Phys. **44,** 1

Korobenko A.., Milner A. A., Milner, V., 2014. Phys. Rev. Lett. **112**, 113004

Kottas, G.S.,Clarke, L.I.,Horinek, D., Michl, J.2005. Chem. Rev. **105**, 1281-1376

Milburn, G.J., 1997, Schrodinger's Machines: The Quantum Technology Reshaping Everyday Life, W. H. Freeman

Nagle, R.K., Saff, E.B., Snider,A.D., 2011. Fundamentals of differential equations, Pearson (8th edition)

Rivas, A., Huelga, S.F., 2011. Open Quantum Systems. An Introduction, SpringerBriefs in Physics, Berlin.

Suzuki Y., Tanimura Y, J. Phys. Soc. Japan **70**, 1167 (2001)

PRVI I DRUGI MOMENT ZA RAVANSKI KVANTNI BRAUNOV ROTATOR U SPOLJAŠNJEM HARMONIJSKOM POLJU

Mi dajemo eksplicitne matematičke izraze za standardna odstupanja i korelacionu funkciju za azimutalni ugao rotacije i njemu kanonski konjugovani moment impulsa ravanskog (jednodimenzionalnog) kvantnog Braunovog rotatora u spoljašnjem harmonijskom potencijalu.Mi uočavamo da postoje neke fizički značajne razlike izmedju pomenutog modela i modela slobodnog rotatora koji je dobro istražen u literaturi.

Ključne reči: *otvoreni kvantni sistemi, kvantno Braunovo kretanje, kvantni rotator*.